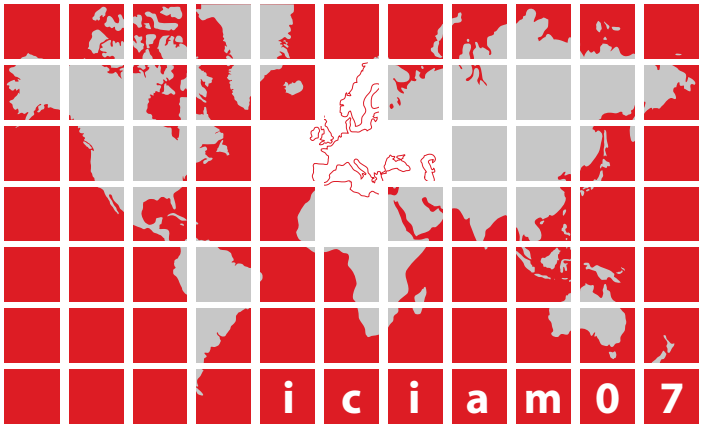
Control of noise-induced behavior in neural network

Abstracts for ICIAM 07

incorporating:

GAMM Annual Meeting 2007
Embedded Meetings
Industry Days



Contents

Embedded Meetings & Industry Days

AMU, Talks

AM/DEM4049/005: **Applied mathematics relevant to Africa.**

Organiser: Jan Persens (University of the Western Cape, South Africa)
Co-organiser: Abderrahman Boukricha (Universite de Tunis El Manar, Tunisia)

In this embedded meeting applied mathematics problems will be presented and tackled which are relevant to Africa. Examples will be the modeling of the spreading of deseases, modelisation of the immune system for responding to malaria parasite plasmodium falcuparum, age-structured epidemic models with vertical transmission and vaccination, mathematical problems related to ecology.

Missing boundary-data recovery and applications. **Amel Ben Abda** (Ecole Nationale d'Ingenieurs de Tunis, Tunisia) AM/TEM4053/005

We consider in this work the problem of recovering missing data on some part of the boundary of a domain from over-specified boundary data on the remaining part of the boundary. This kind of problem occurs often in the engineering sciences, as the reconstruction of physical variables from lacking data is highly useful in many industrial processes. A more common problem, occurring in thermostatics, consists of recovering the temperature in a given domain when the distribution of it and of the heat flux along the accessible region of the boundary are known. Given a flux Φ and the corresponding temperature T on Γ_c, one wants to recover the corresponding flux and temperature on the remaining part of the boundary Γ_i, where Γ_c and Γ_i constitute a partition of the whole boundary $\partial\Omega$. The problem is therefore set as follows:

Find (φ, t) on Γ_i such that there exists a temperature field u satisfying:

$$\nabla \cdot k(x)\nabla u = 0 \text{ in } \Omega, \quad k(x)\nabla u \cdot n = \Phi \text{ on } \Gamma_c, \quad u = T \text{ on } \Gamma_c,$$

where the conductibility field $k(x)$ is real analytic in $L^\infty(\Omega)$. This problem has been known since Hadamard to be ill-posed, in the sense that the dependence of u and consequently of (φ, t) on the data (Φ, T) is known to be not continuous. Two approaches are presented to reconstruct the missing data (φ, t): The first one builds an energy like error functional, the second one resorts to Domain Decomposition tools. These two methods have been successfully numerically experimented for the Laplacian operator.

Applications to the inverse ElectoCardioGraphy (ECG) and ElectroEncephaloGraphy (EEG) probems will be presented.

Population dynamics and epidemic diseases models. **Mohamed El-Doma** (University of Khartoum, Sudan) AM/TEM4070/005

In this talk, we will introduce population models as well as epidemic diseases models. In general there are two main types of models, namely, deterministic models and stochastic models. We only present deterministic models, and concentrate our efforts on structured population models. In particular, we consider populations that are structured either by age, where age is assumed to be the chronological age, that is, the time since birth, or size.

For epidemic diseases models, we concentrate our efforts in age-structured population models where diseases can be transmitted vertically or horizontally or by both modes of transmission, for example, diseases like AIDS, chagas, gonorrhea and hepatitis B are vertically as well as horizontally transmitted, whereas diseases like malaria and tuberculosis are horizontally transmitted. We also consider situations where diseases can cause significant fatalities. It is worth mentioning that such models are seldom considered in the literature, this is partly due to the added mathematical difficulties that arise in such situation. In addition, we introduce vaccination for epidemic diseases models and obtain some conclusions about their eradication.

For size-structured population models, we give some stability results, for the finite size case, which may corresponds to harvesting at specific size, and for the infinite size case.

Modelling the cellular-level interaction between the immune system and viruses. **Gareth Witten** (University of Cape Town, South Africa) AM/TEM4131/005

Mathematical models have shown to provide substantial insights into our understanding of the dynamics of viruses, in particular, the human immunodefiency virus, at both the population and cellular level. Collaboration between experimentalists and mathematical modellers have allowed models to be evaluated and parameterised, and used to test several key hypotheses, for example, the role of the immune system in the progression of the disease and how HIV evolves resistance to antiretroviral treatment. An explosion of the application of mathematical models at the cellular level was seen in the 1980Šs and thus far success in describing HIV and other viruses has been due, in part, to the availability of reliable experimental data. However, there remains a number of puzzling quantitative features. In this presentation I will review the major biological questions being asked and attempt to sketch the development of the mathematical models in this area and how these models have impacted our understanding of HIV pathogenesis in southern Africa.

CSIAM, Talks

CS/DEM4121/015: Industrial and applied mathematics in China.

Organiser: Ya-xiang Yuan (Chinese Academy of Sciences)
Co-organiser: Tatsien Li (Fudan University, PR China)

Inverse heat-transfer problems in steel industry. **Yongji Tan** (Fudan University, PR China) CS/TEM4310/159

In this paper, two problems from the steel industry are discussed. The first one is the control problem for the secondary cooling of continuous casting. The second concerns monitoring the corrosion of the inner wall of the blast furnace and steel ladle. Both problems are formulated as inverse heat-transfer problems and solved by suitable numerical methods. Some theoretic results related to the corrosion problem are obtained.

The generating function of a pricing mechanism for financial derivatives. **Freddy Delbaen** (ETH Zürich, Switzerland), Shige Peng (Shandong Universiity, PR China) CS/TEM4568/159

In this talk we present a theoretical and market-data test of dynamic pricing mechanisms for financial derivatives. A typical model of such a pricing mechanism is the so-called g-expectation defined by solutions of a backward stochastic differential equation with g as its generating function. The Black-Scholes pricing model is a special linear case of this pricing mechanism. We are mainly concerned with two types of pricing mechanisms in an option market: the market pricing mechanism through which the market prices of options are produced; and the ask-bid pricing mechanism operated through the system of market makers. The later one is a typical nonlinear pricing mechanism. Data of prices produced by these two pricing mechanisms are usually quoted in an option market.

We introduce a criteria (i.e., the domination condition) to test whether a dynamic pricing mechanism under investigation is a g-pricing mechanism. This domination condition was statistically tested using CME data documents. The result of the test is significantly positive. We also provide some useful characterizations of a pricing mechanism by its generating function.

Reference:

S. Peng; Modelling Derivatives Pricing Mechanisms with Their Generating Functions, preprint 2006. (arXiv:math.PR/0605599, v1 23 May 2006).

Recent existence results for the multidimensional compressible Navier–Stokes equations. **Song Jiang** (IAPCM, Beijing, PR China) CS/TEM4257/159

Modelling, analysis and numerical simulations are the important aspects in applied mathematics. In this talk we shall concentrate on the analysis aspect of the multidimensional compressible Navier-Stokes equations, which describe the motion of compressible viscous fluids and are a nonlinear hyperbolic-parabolic coupled system. In the last decades significant progress has been made on the mathematical aspect of the Navier-Stokes equations for multidimensional compressible flow. We shall briefly review some recent global existence results on the Cauchy problem with large data. The ideas and developed techniques used in obtaining the global well-posedness will be presented, and some open questions will be discussed.

CS/DEM4121/015: Industrial and applied mathematics in China. #2

Organiser: Ya-xiang Yuan (Chinese Academy of Sciences)
Co-organiser: Tatsien Li (Fudan University, PR China)

(For abstract, see session #1 above.)

Solving a class of constrained black-box inverse variational inequalities. **Bingsheng He** (Nanjing University, PR China) CS/TEM5067/159

Development of computerized tomography in China. **Peng Zhang** (Capital Normal University, PR China) CS/TEM4283/159

X-ray computed tomography (CT) is a one of the great technological achievements in the last century and is critically important for life science, patient care and non-destructive testing in industry, etc. In this rapidly developing field, applied mathematics is a most powerful tool for development of image reconstruction and image processing theory and methods. This talk is a survey of the work on computerized tomography and its applications conducted by Chinese applied mathematicians in the last two decades. It consists of five parts. Part 1 is an overview of the history and development of the research on computerized tomography in China. Part 2 is an introduction of CT theory, scanning configurations, and image reconstruction algorithms. Part 3 is a report on recent achievements by Chinese groups on typical issues in industrial nondestructive testing, including ROI (region of interesting) reconstruction, reconstruction from limited angle data, multiple scanning configurations for large view of field, super-resolution reconstruction, fast implementation of CT reconstruction algorithms, 3D visualization of huge CT data, and virtual design of industrial CT systems, etc. Part 4 are representative applications in medical imaging, material science, nondestructive industrial testing and fossil imaging. Part 5 is a perspective of emerging tomography techniques such as phase-contrast tomography and bioluminescence tomography and future research opportunities. This talk ends with a discussion on the policy for promoting applied and industrial mathematics in China. The presentation is based on the work of collaborators and images kindly provided by other groups in China.

Dynamical modeling based on energy dissipation. **Pingwen Zhang** (Peking University, PR China) CS/TEM4256/159

Energy dissipation for a dynamical model is important not only for the physical correctness but also for stable and robust numerical simulation. In this talk, we introduce a systemic technique for dynamical modeling and a way from energy dissipation law to dynamical equations. We will present a new closure approximation needed for deriving effective macroscopic moment equations from the microscopic FENE kinetic theory modeling viscoelastic polymeric fluids and inhomogeneous kinetic theory of liquid crystal polymers. The simplified system coupling the moment equations and the Navier-Stokes equations still possesses an approximated energy law analogous to the original micro-macro system. Some other examples for complicated coupled models of polymer phase separation and dynamical cell membrane are introduced to expound the whole process. Numerical results show good stability of these models as well as the numerical schemes.

ESMTB Plenary Lecture

ES/IT4124: *Models for cell motility by filament-elongation motors*
Richard Dickinson (University of Florida, USA)

Filament end-tracking proteins, which bind onto and processively advance with elongating cytoskeletal filament ends, play a fundamental and perhaps ubiquitous role in force generation during polymerization of actin filaments and microtubules. These filament end-tracking motors capture energy from nucleoside triphosphate (ATP or GTP) hydrolysis at the filament ends for elongation and force generation by modulating the affinity between end-tracking proteins and filament subunits in a manner that facilitates processive monomer addition and filament end-tracking. Mechanochemical models of force-dependent filament elongation kinetics together with reaction–diffusion–mechanical models of motility demonstrate that the existence of end-tracking motors operating on actin filaments plus-ends can quantitatively explain key observations in various recent studies of actin-based propulsion of particles coated with nucleaction promoting factors (ActA, VASP, N-WASP), such as particle speed, deformations, and saltatory motion.

This work was done in collaboration with Daniel L. Purich, Dept. of Biochemistry and Molecular Biology, University of Florida College of Medicine.

ES/IT3378: *Stochastic modelling of interacting biological populations*
Vincenzo Capasso (Università degli Studi di Milano, Italy)

Particular attention is being paid these days to the mathematical modelling of the social behaviour of individuals in a biological population, for different reasons; on one hand there is an intrinsic interest in population dynamics of swarms, on the other hand agent based models are being used in complex optimization problems (ACOs; i.e. Ant Colony Optimization). Further decentralized/parallel computing is exploiting the capabilities of discretization of nonlinear reaction–diffusion systems by means of stochastic interacting particle systems.

Among other interesting features, these systems lead to selforganization phenomena, which exhibit interesting spatial patterns. Current interest concerns how do properties on the macroscopic level depend on interactions at the microscopic level. Among the scopes of the lecture, a relevant one is to show how to bridge different scales at which biological processes evolve; in particular suitable *laws of large numbers* are shown to imply convergence of the evolution equations for empirical spatial distributions of interacting individuals to nonlinear reaction–diffusion equations for a so called mean field, as the total number of individuals becomes sufficiently large.

In order to support a rigorous derivation of the asymptotic nonlinear integrodifferential equation,problems of existence of a weak/entropic solution will be analyzed. Further the existence of a nontrivial invariant probability measure is analyzed for the stochastic system of interacting particles.

This is work performed in collaboration with M. Burger, D. Morale.

ES/IT3766: *Cell interactions under flow: experiments and modelling*
Claude Verdier (CNRS & Université Grenoble I, France)

We describe the mechanisms which rule the different laws governing cell–cell interactions, in particular when leukocytes or cancer cells interact with the endothelium under flow conditions. These mechanisms can lead to cell rolling and extravasation. Important issues concern cellular adhesion, cell microrheology, the influence of shear stresses, and mechanotransduction.

Experiments are performed to understand these features using microrheology techniques[1], as well as flow chambers to investigate cell–cell interactions. Different behaviors are exhibited[2], in which cancer cells show totally different behaviors; they either intermingle within the endothelium and form mosaic monolayers, or disappear at cell–cell junctions (i.e., extravasation).

Different processes such as kinetic models or stochastic ones can be used to include the adhesion effects. Biochemical bonds can be formed or broken in a probabilistic way or through kinetic reactions. This is included in a 3D model of a cell interacting with a rigid wall[3]. The cell is considered as a viscoelastic composite object surrounded with a membrane with cortical tension. Simulations have been compared with experiments involving the rolling of leukocytes on the endothelium.

[1] Canetta, E., Leyrat, A., Verdier, C. and Duperray, A; Measuring cell viscoelastic properties using a force spectrometer: influence of the protein–cytoplasm interactions. Biorheology, 42(5), (2005) pp.321–333.
[2] Chotard-Ghodsnia, R., Haddad, O., Leyrat, A., Drochon, A., Verdier, C. and Duperray, A.; Morphological analysis of tumor cell/endothelial cell interactions under shear flow. J. Biomechanics, 40(2), (2007) pp.335–344.
[3] Jin, Q., Verdier, C., Singh, P., Aubry, N., Chotard-Ghodsnia, R. and Duperray, A.; Direct simulation of the migration of leukocytes in pressure driven flows. submitted (2006).

ESMTB, Talks

ES/DEM4883/000: **Cell dynamics and ECM interactions.**
Organiser: Luigi Preziosi (Politecnico di Torino, Italy)
Co-organiser: Wolfgang Alt (Universität Bonn, Germany)
Co-organiser: Andreas Deutsch (TU Dresden, Germany)

Cellular traction as an inverse problem. **Davide Ambrosi** (Politecnico di Torino, Italy) ES/TEM3323/120

The evaluation of the traction exerted by a cell on a planar substrate is here considered as an inverse problem: shear stress is calculated on the basis of the measurement of the deformation of the underlying gel layer. The adjoint problem of the direct two-dimensional plain stress operator is derived by a suitable minimization requirement. The resulting coupled systems of elliptic partial differential equations (the direct and the adjoint problem) are solved by a finite element method and tested vs. experimental measures of displacement induced by a fibroblast cell traction.

Continuum model of cell adhesion and migration. **Esa Kuusela** (Universität Bonn, Germany), Wolfgang Alt (Universität Bonn, Germany) ES/TEM4152/120

Certain types of cells (e.g., *keratinocytes*), have the ability to move on surfaces with appropriate adhesive coating. Modeling the complicated intra-cellular processes generating this motion forms an intriguing challenge to the mathematical biologists. The essential cell functions for motion are at least the continuous polymerization, depolymerization and deformation of intra-cellular actin filament network, as well as the evolution of cell membrane protein structures that can mediate the network generated forces to the underlying surface.

We will here describe a large-scale continuum model capable of treating these microscopic processes. The 2-dimensional model consists of two layers. The top layer describes the interior of the cell as a two-phase fluid where the components are the highly viscous dynamic filament network and the low viscous intra-cellular liquid, the cytosol. The bottom layer consist of the cell membrane and the discrete focal adhesion cites.

The presented model realistically handles the polymerization, depolymerization and flow of filament network in whole cells and cell fragments. We will also show that this simple model is able to show many of the characteristics of moving keratinocytes like rapid protrusion and retrograde flow of actin filaments.

A comparison of chemotaxis *models.* **Thomas Hillen** (University of Alberta, Canada) ES/TEM3401/120

Macroscopic models for chemotaxis are partial differential equations with cross diffusion and are of Keller-Segel type. Various versions of the Keller-Segel model have been used in the literature for various purposes. In this talk I will review and compare different subclasses which I roughly classify into eight categories: 1. classical, 2. receptor binding, 3. volume filling, 4. saturation in the chemotactic sensitivity, 5. non-local gradient sensing, 6. nonlinear diffusion, 7. saturation in the chemical signal, and 8. population kinetics.

For each of these model classes I will present applications, review results on local and global existence, and discuss pattern formation. It turns out that coarsening of pattern is a common property of all these models. We demonstrate this numerically (joint work with K. Painter, Edinburgh).

ES/DEM4884/000: Dynamics of cell populations.

Organiser: Wolfgang Alt (Universität Bonn, Germany)
Co-organiser: Luigi Preziosi (Politecnico di Torino, Italy)
Co-organiser: Andreas Deutsch (TU Dresden, Germany)

Cellular automaton modelling of spatio-temporal pattern formation in interacting cell systems. **Andreas Deutsch** (TU Dresden, Germany) ES/TEM4329/120

Examples of spatio-temporal pattern formation are life cycles of bacteria and social amoebae, embryonic tissue formation, wound healing or tumour growth. Thereby, development of a particular spatio-temporal "multi-cellular" pattern may be interpreted as cooperative phenomenon emerging from an intricate interplay of local (e.g. by adhesion) and non-local (e.g. via diffusing signals) cell interactions. What are cooperative phenomena in interacting cell systems and how can they be studied?

Mathematical models are required for the analysis of cooperative phenomena. Typical modeling attempts focus on a macroscopic perspective, i.e. the models (e.g. partial differential equations) describe the spatio-temporal dynamics of cell concentrations. More recently, cell-based models have been suggested in which the fate of each individual cell can be tracked. Cellular automata are discrete dynamical systems and may be utilized as cell-based models.

Here, we analyze spatio-temporal pattern formation in cellular automaton models of interacting discrete cells. We introduce lattice-gas cellular automata and a cellular automaton based on an extended Potts model that allows to consider cell shapes. Model applications are bacterial pattern formation and tumour growth.

From single cells to tissue architecture: a bottom-up approach to modelling the spatio-temporal organisation of complex multicellular systems. **Joerg Galle** (Universität Leipzig, Germany), Dirk Drasdo (University of Warwick, UK) ES/TEM4133/120

Collective phenomena in multi-cellular assemblies can be approached on different levels of complexity. Here, we review a number of mathematical models which consider the dynamics of each individual cell; so called individual cell-based models (IBMs). As a special feature, these models allow to account for intracellular decision processes, triggered e.g. by biomechanical cell-cell or cell-matrix interactions. Consequently, they allow studying the impact of regulatory malfunction on the growth and homeostasis of the assembly under consideration. This is achieved assuming that the intracellular processes act on a limited number of effective cell-biological and biophysical parameters. In the case that these parameters are experimentally accessible, IBMs can reach a stage where they may contribute to unveil the processes that underlie the organization of tissues and multicellular aggregates. The applications discussed here range from regulation of growth and contraction of in vitro cell populations to cell-contact dependent regulation of tumor morphology.

Periodic hematological disease: insight into origins derived from mathematical modeling. **Michael Mackey** (McGill University, Canada) ES/TEM3329/120

There are a variety of periodic hematological diseases such as cyclical neutropenia, cyclical thrombocytopenia, and periodic leukemia. Each presents their own difficulties to the mathematical modeler in terms of trying to deduce the possible origins of the abnormal dynamics and suggesting treatment methods. This talk will focus on these issues using selected diseases as case studies.

ES/DEM1219/010: Subcellular dynamics.

Organiser: Andreas Deutsch (TU Dresden, Germany)
Co-organiser: Luigi Preziosi (Politecnico di Torino, Italy)
Co-organiser: Wolfgang Alt (Universität Bonn, Germany)

The purpose of the European Society for Mathematical and Theoretical Biology is to promote the development of theoretical approaches and mathematical tools in biology and medicine which has an undisputable medical, industrial and social interests.

Insights and predictions from mathematical modelling are used increasingly in decision support in medicine (e.g. immunology and spread of infectious diseases, cancer research, cardio-vascular research, neurological research, optimisation of medical treatments, imaging). The research trend is now to look at the phenomena occurring at the cellular and subcellular scales, e.g., cell motion and behaviour, signal transduction, genomics, proteomics.

In this respect this embedded meeting has as its goal to foster interdisciplinary collaboration between mathematicians and bioscientists and to act as a forum for the presentation of recent research results and new research directions in computational cell biology.

Systems biology towards life in silico*: mathematics of the control and regulation of living cells.* **Hans Westerhoff** (Vrije Universiteit Amsterdam, The Netherlands) ES/TEM5037/120

Systems Biology is the science that discovers general principles underlying the emergence of biological function from the interactions of components of living systems. By specifying in a <91>silicon cell<92> the dynamic ways in which macromolecules interact, the emergent properties can be calculated through numerical mathematics. This approach is on its way towards the calculation of more and more of living organisms in the computer. These silicon cells help discover new principles of Life by induction, providing a new route, parallel to empirical Biology, and similar to computational physics. They also enable differential network-based drug design.

Much of Biology progresses as an empirical science where discoveries are made by experimental testing of hypotheses. By abstracting the ways macromolecules <91>listen<92> and <91>talk<92> to each other in living cells, a set of elemental properties can be formulated for living organisms. These then enable the deduction through mathematics of principles that are important for control and regulation of the vital fluxes of living cells. The simplest of these will be illustrated, for the control, regulation and robustness of fluxes, of oscillations and of signal transduction relevant for cancer.

Modelling asymmetric division in the early C. elegans *embryo.* **François Nédélec** (EMBL, Heidelberg, Germany) ES/TEM4272/120

Interactions between microtubules fibers and the cell cortex play a critical role in positioning organelles in a variety of biological contexts. In *C. elegans*, for example, cortical forces acting on microtubules originating from the spindle-poles displace the mitotic spindle towards the posterior in response to polarity-cues. Using EBP::GFP and YFP::tubulin we observed that microtubules shrink soon after touching the cortex. From this, we proposed that cortical adaptors mediate microtubule depolymerization energy into pulling forces. We then used stochastic computer simulations to show that such force production mechanism is crucially determined by the assembly/disassembly dynamics of fibers and their mechanical properties. Furthermore, we show that these simulations reproduce faithfully anaphase spindle oscillations and posterior displacement in 3D.

Automated analysis of spatio-temporal cell microscopy images: classification, tracking, and registration. **Karl Rohr** (Universität Heidelberg, Germany), Nathalie Harder (Universität Heidelberg, Germany), Roland Eils (Universität Heidelberg, Germany) ES/TEM4835/120

The effectiveness of large-scale and high-content cellular screening techniques in biological applications significantly depends on the analysis of the acquired image data. Because of the enormous increase in the generation of 2D, 3D, and 4D microscopy images a manual evaluation is no longer possible and a computer-based analysis is necessary.

We have developed an image analysis approach for the evaluation of large-scale cell phenotype screens generated by high-throughput RNAi experiments. Based on confocal fluorescence microscopy cell-array images the task is to determine the influence of genes on the process of cell division and thus to identify gene function. Our approach allows to automatically segment and classify cell nuclei into different cellular phenotypes. The segmentation of cells is based on an efficient region-adaptive thresholding scheme. For cell classification we employ support vector machines using a large spectrum of image features. We have also developed a tracking scheme which exploits the temporal information in consecutive time-lapse images and thus enables to compute the ancestral relationships between cells.

Another central task in biological image analysis is the normalization of cell microscopy images for subsequent quantification and statistical analysis of the cell structure. To this end a geometric transformation needs to be computed. The task of finding an optimal geometric transformation between corresponding image data is known as image registration and generally one has to use non-rigid (elastic) deformation models. We have developed elastic registration approaches for image normalization and have successfully applied them to multi-channel confocal cell nucleus images.

Aircraft Design, Talks

AD/DID430/061: **Numerical optimization for industrial aircraft design.**

Organiser: Nicolas Gauger (HU Berlin & DLR Braunschweig, Germany)
Co-organiser: Norbert Kroll (DLR Braunschweig, Germany)
Co-organiser: Klaus Becker (Airbus Deutschland GmbH, Germany)

The workshop is organized by the Pilot Center Germany North of ERCOFTAC and aims to bring together research scientists from universities, research institutes and industry that work in the field of aerodynamic shape optimization. The requirements for practical shape optimization will be worked out, new solution approaches and optimization tools from research institutes will be presented in conjunction with innovative ideas from the forefront of mathematical research at universities. Particular attention will be paid to the fact that aerodynamic shape optimization is a part of a larger, multi-disciplinary design process.

Numerical optimization for industrial aircraft design at Airbus. **Murray Cross** (Airbus, UK) AD/TID4524/061

There is an ever increasing requirement to improve the performance and cost effectiveness of commercial aircraft due in a competitive marketplace with multiple external constraints. Looking back at history we see tremendous strides in efficiency and effectiveness of such commercial aircraft, enabled by improving technology, tools, processes and knowledge. This optimisation process is a fundamental part of an aerospace engineers approach, and part of the natural ability to look at different approaches and selecting the best technique for applying to the job in hand. In recent times and certainly in the future, a combination of the complexity of the engineering system, the requirement to attain higher and higher levels of performance, and the increased technical capability, has lead to the introduction of numerical optimisation techniques coupled with high fidelity engineering analysis.

This presentation will review the need for optimisation, the key technologies enabling such techniques, and applications for such techniques in an Airbus Engineering context, with a focus on aerodynamics.

Status and challenges of aeroshape design of future aircrafts. **Phillipe Rostand** (Dassault Aviation, France) AD/TID4525/061

Aeroshape design of aircrafts is a continuously evolving process; very significant progresses have been made in the last ten years and a high degree of maturity has been reached. Most of the elements of the arodynamics of conventional fighter aircrafts or business jets are modeled and understood to a degree, and so can be the object of reasonably deterministic design processes. Consequently innovative designs have been obtained which could not have been derived earlier, and large efficiency gains in the design process have been observed. Progresses have been obtained combining research efforts of industry, research centers and academia; a summary of recent results for business jet design is presented. However new challenges have appeared that call for further evolution of processes, on which current research efforts are focused. New challenges come primarily from: New environmental requirements, which call for significant changes in business jet design, with community noise reduction a first level objective if ACARE targets are to be met, Stealth requirements, to be fully integrated in combat manned and unmanned aircraft design processes. New competitivity requirements, both on performances, in particular on aircraft speed, with the Supersonic Business Jet, and on recurring and non-recurring costs, Risk reduction requirements, in particular in the much shortened design phases.

Experiences in aerodynamic shape optimization at EADS-military aircraft systems. **Herbert Rieger** (EADS Military Air Systems, Germany), Norbert Kroll (DLR Braunschweig, Germany), Klaus Becker (Airbus Deutschland GmbH, Germany) AD/TID4526/061

In recent years the numerical aerodynamic simulation methodology has demonstrated the enormous potential by which that technology can contribute to improvements of aircraft design during almost all stages of aircraft development. This has fostered the use of advanced optimization techniques for complex aerodynamic shape design which involves also multidisciplinary considerations. Presently the aerospace industry has the choice over a wide range of different optimization algorithms which rely e.g. on gradient-based, evolutionary and genetic optimization algorithms. The approach taken is to identify for the specific problem at hand the best suited optimization technique offered in a general multiobjective design optimization environment which allows easily organizing and adapting the necessary work flow. Over the years EADS Military Aircraft Systems has developed, implemented and automated all process elements to build up an advanced design and optimization capability based on a parametric CAD geometry modeling approach for providing the geometry models suitable for an automated unstructured mesh generation system as well as a flexible flow simulation system which handles all kind of steady or unsteady RANS flow problems with and without moving boundaries. The results of the approach on various optimization problems are presented ranging from simpler 2D aerodynamic problems up the multi-point and multi-objective optimization of full aircraft configurations as a multi-disciplinary approach including structural considerations and requirements.
N. Kroll, K. Becker, H. Rieger, F. Thiele "Ongoing Activities in Flow Simulation and Shape Optimization within the German MEGADESIGN project", ICAS Proceedings 2006, Paper 2006-3.11.1

AD/DID430/061: **Numerical optimization for industrial aircraft design.** #2

Organiser: Nicolas Gauger (HU Berlin & DLR Braunschweig, Germany)
Co-organiser: Norbert Kroll (DLR Braunschweig, Germany)
Co-organiser: Klaus Becker (Airbus Deutschland GmbH, Germany)

(For abstract, see session #1 above.)

Novel techniques for aerodynamic design optimization. **Volker Schulz** (Universität Trier, Germany) AD/TID4527/061

Aerodynamic design is an engineering issue of high economic importance. Often, tedious experimental as well as numerical studies are involved. In a collborative effort of DLR Braunschweig and University of Trier, new mathematical tools have been developed, which can speed up the design process enormously from a computational point of view. The talk will discuss the theoretical and the practical asepcts of these techniques which are based on one-shot methods.The robust treatment of model unsecurities pose additional challenges and will play a role, too.

Theory and practice of optimal shape design for fluids. **Bijan Mohammadi** (Université Montpellier II, France), Olivier Pironneau (Université Paris VI, France) AD/TID4528/061

This is a survey of some recent developments in Optimal Shape Design (OSD) for fluids. Existence, sensitivity, compatibility of discretizations as well as efficient algorithmic implementations with low complexity are critical. We discuss some of these issues with application to shape optimization for aerodynamic noise reduction in supersonic (sonic boom) and subsonic regimes (noise due to aerodynamic unsteadinesses).

Coupling of sizing optimization and topology optimization for industrial aircraft design. **Joachim Gwinner** (Universität der Bundeswehr München, Germany) AD/TID4529/061

In structural aircraft design as well as in other applications of light weight design it is important to optimize simultaneously all load bearing members of a structure, like skin, stringer, longerons and frames,

in one optimization loop. Very often, sizing optimization with respect to member size or thickness has been separately applied to the single low dimensional members; e.g., to the skin modelled by shell elements or the longereons, modelled by beam elements, respectively. On the other side, stand alone topology optimization with respect to the density as design variable has been applied to single frames to find the relevant load paths and an optimal material distribution. Clearly, a direct numerical treatment of the total structure based on a complete FE discretization leads to large (although sparse) linear systems that have to be called for and solved by Gauss-Cholesky factorization within the optimization loop and is thus prohibitive in view of a plentitude of different loading cases and failure modes.

In contrast, during the last decade, iterative domain decomposition methods have become a major tool in numerical analysis of partial differential equations. Such methods kave been more recently[1,3] invented and studied in the foreward analysis of coupled ODE-PDEs. Moreover domain decomposition methods have also been developped for the optimal control of PDEs on multi-linked or networked domains[4]. Finally at the infinite-dimension level, structural optimization, in particular topolgy optimization can be seen[2] as a problem of control in the coefficients.

It is obvious from the physical point of view that such decompositions should respect the structural members as individuals coupled at multiple joints. Thus we seek the decoupling of multiple joint conditions or, put in other words, a nonoverlapping domain decomposition procedure, what in engineering terminology can be labelled as a substructuring approach. Here in this contribution we concentrate to coupled 1D/2D structures (beam/plane linear elasticity) and develop iterative domain decomposition methods in structural optimization.

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Electromagnetics, Talks

EL/DID1032/015: Challenges in computational electromagnetics.

Organiser: Ralf Hiptmair (ETH Zürich, Switzerland)

Electromagnetic phenomena are at the heart of almost every modern technology. Thus, their accurate and fast numerical simulation becomes a key capability in industrial research and development, as computer aided design and testing assumes a central role in product development. The core task in electromagnetic simulation boils down to the approximate solution of boundary value problems arising from Maxwell's equations. This bland description conceals a host of really challenging problems. Important issues concern the proper discretization both in a finite element and boundary element framework, the robustness of the methods with respect to small wavelengths, the design of fast and robust iterative solvers, the incorporation of sources and lumped devices, to name only a few. Mathematics has contributed significantly to tackling these issues, and will continue to play a crucial role as rapid advances of technology and increasing computer power raise fresh challenges.

This industry day will make it possible to catch a glimpse of some current issues confronted in industrial electromagnetic simulations. For some of the problems state of the art numerical techniques will be addressed, others may still be far from being solved. Thus, practitioners will be updated on modern numerical methods and researchers can get inspiration on new and relevant topics. Thus, attending the industry day lectures will be worth while for a wide range of people.

Numerical simulation of electromechanical systems: some trends and accomplishments. **Stefan Kurz** (Universität Frankfurt, Germany) EL/TID4908/015

For the development and optimization of electromechanical systems and their components numerical modeling and simulation have become indispensable tools. Numerical methods like the Finite Element and the Boundary Element method are widely used in industry. Since the requirements regarding level of details and accuracy of the models are continuously increasing, fast methods are of particular interest. Robust matrix compression techniques, both for modeling at an appropriate accuracy level as well as construction of preconditioners have gained momentum recently. In this presentation, the theoretical foundations are briefly reviewed, including the connection to the so-called Discrete Exterior Calculus. A solenoid actuator for Diesel injection and a claw pole alternator are considered as examples, and the usefulness of symmetry exploitation and matrix compression techniques is pointed out. Finally, some trends and open issues are reported, in order to stimulate further research and industry collaborations.

Mathematical challenges for commercial high-frequency electromagnetic simulation tools. **Peter Thoma** (Computer Simulation Technology, Germany) EL/TID4909/015

The design of high speed electronic devices becomes less and less feasible without the efficient application of electromagnetic simulation techniques. Increasing packaging densities demand for robust full three dimensional solutions which require the application of general finite element, boundary element or finite difference techniques. Those methods typically lead to huge systems of equations with many millions of unknowns which need to be solved without user interaction. A close cooperation between software developers and mathematical research groups is essential in order to provide state-of-the-art solutions for these challenging problems. The talk will provide an overview of a number of industrial applications together with the currently applied corresponding solver technology. Finally a short summary of open mathematical challenges will be given which should provide some links to potential cooperation areas.

High-order scattering solvers and surface representation algorithms. **Oscar Bruno** (California Institute of Technology, USA) EL/TID4887/015

I will consider algorithms and methodologies for the numerical solution of problems of scattering by complex bodies in three-dimensional space, and I will focus on a newly developed class of high-order algorithms for these problems. These methods, which are based on integral equations, high-order integration, fast Fourier transforms and highly accurate high-frequency methods, can be used in the solution of problems of electromagnetic and acoustic scattering by surfaces and penetrable scatterers, even in cases in which the scatterers contain geometric singularities such as corners and edges. In all cases the solvers exhibit high-order convergence, they run on low memories and reduced operation counts, and they result in solutions with a high degree of accuracy. In this talk I will describe the basic methodologies inherent in these approaches. In particular, I will touch upon a new class of high-order surface representation methods introduced recently which, starting from point clouds or CAD data, can produce high-order-accurate surface parametrizations and associated surface/volume finite-element representations, suitable for high-order numerical simulations, of complex engineering surfaces in three-dimensional space.

Numerical challenges in the simulation of electrical arcs. **Henrik Nordborg** (ABB Corporate Research, Switzerland) EL/TID5017/159

The electrical arc is important in many technical applications, both for providing basic functionality (arc furnaces, plasma torches, arc welding) or as an unwanted result of electrical breakdown. The numerical simulation of arcs in real engineering application is difficult for a number of reasons. First, the three-dimensional geometries are complex enough to make a pure electromagnetic or flow simulation challenging. Secondly, the electromagnetic solver has to cope with the coupling to the gas flow, huge differences in electrical conductivity, and, in particular, continuously vanishing conductivity at the edge of the arc. Finally, the problems are always transient, requiring of the order to 10'000 time steps per simulation. The presentation will outline the main numerical challenges of this problem, with special emphasis on the electromagnetic part.

Food Processing, Talks

FP/DID3954/151: Simulating flows in food processing.

Organiser: Franz Tanner (Michigan Technological University, USA)
Co-organiser: Erich Windhab (ETH Zürich, Switzerland)
Co-organiser: Marco Dressler (ETH Zürich, Switzerland)

Deformation, orientation and breakup of droplets in flows. **Kathleen Feigl** (Michigan Technological University, USA) FP/TID4693/156

Immiscible multiphase fluid systems, such as emulsions and polymer blends, are encountered in manufacturing processes in a variety of industries. In particular, in dispersing processes, droplets of one fluid are oriented, deformed and broken up in another fluid. The properties of the final product depend, in part, on the shape, orientation and size distribution of the disperse phase droplets. In this talk, the orientation, deformation and breakup behavior of viscous droplets under various flow, fluid and interfacial conditions is discussed. The focus is on the effect of the imposed flow type or dispersing device, the viscosity ratio, the capillary number (ratio of viscous forces to interfacial tension) and, in the presence of surfactants, surface gradients in interfacial tension (e.g., Marangoni stresses). Results are presented from both numerical simulations and experiments.

Relationship between rheology and microstructure of emulsion systems in an extrusion flow. **André Braun** (ETH Zürich, Switzerland), Marco Dressler (ETH Zürich, Switzerland), Erich Windhab (ETH Zürich, Switzerland) FP/TID5046/156

Recently, a mathematical model describing polymer blends with droplet morphology was derived within the framework of non-equilibrium Thermodynamics by Dressler and Edwards[1]. The model allows to predict the difficult interplay between fluid dynamics, droplet morphology and the non-linear viscoelastic properties of the blend. The complex set of nonlinear, coupled differential equations are solved computationally for a mixed Couette/Poiseuille flow as encountered in the metering section of a single screw extruder. In our code we consider both the mixing flow perpendicular to the flights of the extruder and the conveying flow parallel to the flights. We have performed calculations for different model (e.g., blend component viscosity ratio) and flow geometry parameters (e.g., helix angle of the extruder screw). Macroscopic flow characteristics such as the volumetric throughput, the residence time distribution function, and the non-Newtonian flow stresses are discussed along with microscopic characteristics of the blend such as oblate/prolate configurations of the droplets, break-up/coalescence rates, and matrix micro-structural characteristics.

The results from this modeling / simulation approach have been applied in order to investigate correlations with partial coalescence phenomena of fat globules in ice cream extrusion processing.

[1] Dressler, M. and Edwards, B.J.; Rheology of polymer blends with matrix-hase viscoelasticity and a narrow droplet size distribution. J. Non-Newtonian Fluid Mech., 120 (2004) pp.189–205.

General Session 1 Topic Discussion. **Marco Dressler** (ETH Zürich, Switzerland) FP/TID5048/156

FP/DID3954/151: Simulating flows in food processing. #2

Organiser: Kathleen Feigl (Michigan Technological University, USA)
Co-organiser: Erich Windhab (ETH Zürich, Switzerland)
Co-organiser: Marco Dressler (ETH Zürich, Switzerland)

(For abstract, see session #1 above.)

Design of static mixing reactors by CFD. **L Moser** (ProCeng Moser GmbH, Switzerland) FP/TID5052/156

Auslegung von Misch-Reaktoren mittels CFD

In der Kunststoffchemie werden CSE-XR Mischreaktoren der Firma Fluitec Georg AG eingesetzt. In diesen Reaktoren werden Kunststoffschmelzen innig gemischt, polymerisiert und die entstandene Wrme wird abgeführt. Die Reaktoren stehen unter einem Betriebsdruck von ber 250 bar. Die Polymerschmelzen verhalten sich strukturviskos. Messungen der abgeführten Wärme, der Verweilzeit sowie die Mischeigenschaften sind schwierig. Mittels CFD Simulationen konnten Reaktoren mit verschiedenen Grössen für unterschiedliche Polymerschmelzen untersucht und ausgelegt werden.

Eine Herausforderung stellt dabei die Beschreibung des Viskosittsverhaltens sowie die Grsse der Modelle dar. Das Produkt ändert seine Viskosität in Funktion der Scheerrate und der Temperatur.

Die Netze umfassen mehr als 22'000'000 Zellen. Das Viskositätsverhalten des Produktes wurde mittels UDF's gelöst. Die Simulationen werden auf dem Linux Cluster mit mehreren CPU's der ProcEng Moser GmbH durchgeführt.

Viscous and non-Newtonian mixing processes: what can CFD bring?. **Philippe Tanguy** (École Polytechnique de Montréal, Canada), Mourad Heniche (École Polytechnique de Montréal, Canada) FP/TID5047/156

This paper will highlight the capabilities and advantages of the virtual finite element method based on the fictitious domain method with distributed Lagrangians to tackle mixing problems involving complex kinematics, multiple impellers and non-Newtonian rheologies. Three examples will be discussed, namely two Multi-Shaft Mixer technologies, i.e. the dual shaft concentric coaxial mixer and the dual shaft eccentric mixer, and one example of a Single-shaft Multifunctional Impeller Mixer, namely the Maxblend technology from Sumitomo.

The presentation will be divided in two parts: a theoretical section dealing with an up-to-date summary of the most recent variational formulation, discretization techniques and algorithms, and an application section where the performance of the mixers will be thoroughly analyzed based on the above methods. Results will be compared with experimental data showing the usefulness of the numerical approach to handle complex mixing problems.

Modeling and simulation of sprays in food processing. **Franz Tanner** (Michigan Technological University, USA) FP/TID4716/156

Sprays are widely used in food processing, usually to produce a powdered substance with particular properties. Sprays consist of liquid and/or solid particles which move in a gaseous environment. They are modeled as dispersed multiphase flows in the turbulent flow regime, where the dispersed particles interact with each other and the environment, and undergo phase changes. This complex state of affairs is described by a set of differential equations together with appropriate state equations and initial and boundary conditions.

The gas phase is described with the three-dimensional Reynold–Favre-averaged conservation equations for species, mass, momentum and energy, in combination with a turbulence model. The liquid phase is formulated as a stochastic evolution law of the normalized particle flux which is governed by the various phenomena such as particle–particle and particle–gas interactions, as well as phase changes such as solidification and/or evaporation. In order to describe properly these processes, the change in the spray state variables, given by the particle position, velocity, temperature, size and deformation parameters, is determined by sub-models involving the aforementioned particle–particle and particle–gas interactions, subject to initial and boundary conditions for the particle states.

The coupling between the dispersed phase and the gas phase is achieved by means of appropriate source terms in the gas equations. These source terms are obtained from the spray variables by integration of the mass, momentum and energy values over all particles at a given position and time.

In this talk, an overview of today's state-of-the-art spray modeling will be presented, and various modeling aspects, including validations with experimental data, will be discussed. Further, results from spray simulations of real-world problems will be presented.

General Session 2 Topic Discussion. **Marco Dressler** (ETH Zürich, Switzerland) FP/TID5049/156

Pharmaceutics, Plenary Talk

PH/IT4994: *Does a rational way for designing a blockbuster drug exist?*
Walter Schilling (Hoffman-La Roche, Switzerland)

Current strategies and processes for designing drugs, hopefully blockbusters, are reviewed and supported by actual examples within a historical context.

Pharmaceutics, Talks

PH/DID4323/015: **Predicting the blockbuster in pharmaceutical design.**
Organiser: Gerd Folkers (Collegium Helveticum, Switzerland)

Simulation of how a drug molecule interact with its counterpart in the body, usually termed *receptor*, has been one of the major interests in pharmaceutical research over the last three decades. Meanwhile the simulation techniques have reached certain sophistication at the molecular level, due to fast computers, fast algorithms and fast high-resolution spectroscopy. Hence, useful attempts are made to investigate the drug's fate and the body's response at a very early stage of the drug development process in virtual space. The more knowledge is gained before the new chemical entity enters the clinics, the ore precise, predictive and safer the clinical studies and the lower the attrition rate will be.

The term blockbuster usually describes a drug whose global turnover exceeds one billion USD and marks the goal of development of new drugs by the large pharmaceutical companies. However, prediction tools for living systems, are necessarily reductionistic and expensive complementary sets of experiments are indispensable. Therefore, new simulation technologies to understand the phenomenon of molecular similarity in respect to biological activity, to cover specificity of drug-receptor interaction and in parallel help to understand closely-related drug toxicity are the front-line of research.

Predicting the next blockbuster: in silico *techniques for bio-activity profiling of drug candidates.* **Thierry Langer** (Inte:Ligand, Austria) PH/TID4882/159

In silico or virtual screening has gained a high impact for the efficient discovery of novel potential bio-active compounds in modern pharmaceutical research. The concept of chemical feature-based pharmacophore models has been established as state-of-the-art technique for characterizing the interaction between a macromolecule and a potential ligand. While in ligand-based drug design, feature-based pharmacophore creation from a set of bio-active molecules is a frequently chosen approach, structure-based pharmacophores are still lacking the reputation to be an alternative or at least a supplement to docking techniques. Nevertheless, 3D pharmacophore screening bears the advantage of being faster than docking and to transparently provide the user with the relevant information that is used by the screening algorithms to characterize the ligand-macromolecule interaction. As an extension of such an approach, we have successfully introduced parallel pharmacophore-based screening as an in silico method to predict the potential biological activities of compounds by screening them with a multitude of pharmacophore models. We present an overview of our technology together with the results of an application example employing a set of antiviral compounds that were submitted to in silico activity profiling using our pharmacophore building platform LigandScout. The results of the screening experiments show a clear trend towards correct prediction of activity profiles.

The challenge of predicting drug toxicity in silico. **Angelo Vedani** (Biographics Laboratory 3R, Switzerland) PH/TID4438/159

Poor pharmacokinetics, side effects and compound toxicity are frequent causes of late-stage failures in drug development. A safe in silico identification of adverse effects triggered by drugs and chemicals would be highly desirable as it not only bears economical potential but also spawns a variety of ecological benefits: sustainable resource management, reduction of animal models and possibly less risky clinical trials. In computer-aided drug discovery, both existing and hypothetical compounds may be studied; the methods are fast, reproducible, and typically based on human bioregulators, making the question of transferability obsolete. In the recent decade, our laboratory contributed towards the development of in silico concepts (automated flexible docking, multi-dimensional QSAR) and validated a series of "virtual test kits" based on the estrogen, androgen, thyroid, aryl hydrocarbon, glucocorticoid and peroxisome-proliferator activated receptor (endocrine disruption, receptor-mediated toxicity) as well as on the enzyme cytochrome P450 3A4 (metabolic transformations, drug-drug interactions). The test kits are based on the three-dimensional structure of their target protein or a surrogate thereof and were trained on a representative selection of 538 substances. The underlying 6D-QSAR technology is based on a genetic algorithm and a directional force field. Subsequent evaluation of 157 compounds different therefrom showed that binding affinities are predicted close to experimental uncertainty. These results suggest that our approach is suited for the in silico identification of adverse effects triggered by drugs and chemicals and encouraged us to compile an Internet Database for the virtual screening of drugs and chemicals for adverse effects. Details and results can be found under http://www.biograf.ch/index.php?id=projects

Computational approximations for large and complex biochemical processes. **Markus Hegland** (Australian National University), Kevin Burrage (University of Queensland, Australia) PH/TID4941/159

Computational investigations of stochastic biochemical processes require the computation of features like moments, correlations and modes. While these features can be obtained using a statistical investigation of repeated simulations they are directly obtained from the finite dimensional probability distributions which characterize the stochastic process. However, any attempt to determine these probability distributions faces the challenge posed by the extreme size of the state space of biochemical systems which is a consequence of the curse of dimensionality. We will discuss some approximations which can be applied to deal with this challenge. In particular we reduce the size of the state space by aggregating groups of states into a single state and we address the curse of dimensionality using a sparse grid approximation. Using this approach we have been able to model a simple gene regulatory cascade with 100 protein species.

The whys and hows of stochastic modelling of biochemical systems. **Kevin Burrage** (University of Queensland, Australia) PH/TID4937/159

Noise is a fundamental phenomenon in many biological systems including gene regulation. Noise can adversely affect cell function but it can also be a source of robustness, signal amplification and selection of signalling pathways. In this talk we discuss how intrinsic noise can be modelled in biochemical systems via the use of nonlinear discrete Markov processes. We will also show how delay, vital in the modelling of transciption and translation, can be put into this framework. We will illustrate these ideas through two applications: the MAPK cascade (which can be viewed as a multiscale model, linking the plasma membrane and the cytosol) and the Hes1 gene as a molecular switch (viewed as a fine scale model with delay and intrinsic noise).

Risk Management, Plenary Talks

RM/IT4861: *In full swing: optimizing portfolios of flexible gas contracts*
Oleg Zakharov (Lacima Group, UK)

After presenting a brief history of gas markets and the origin of swing contracts we discuss realistic examples of swing contracts and Stochastic Dynamic Programming approaches in optimizing a single swing contract. Further topics treated are the importance of hedging in forward markets and liquidity considerations and the value optimization conditional on limited risk.

RM/IT4857: *Generation of consistent market and credit scenarios: the calibration of a geometric model*
Simone Farinelli (UBS, Switzerland)

A scenario generator for both market and credit risk drivers is developed. On the basis of historical data, financial time series are projected into the future. The foundations were given in 1998 by Andrew Smith, who developed a coherent mathematical framework applicable to all stochastic investment models, allowing for features commonly believed to be essential and/or desirable: positive interest rates, mean reversion (where appropriate), full term structures, efficient markets, absence of arbitrage. The model consists of two parts:

- a geometrical part, where the concepts of gauge, deflator and term structure for every quantity modelled is introduced; and
- a stochastic part, where a stochastic model is applied to a minimal set of gauges (called *principal gauges*) to generate the scenario simulations.

The stochastic part is calibrated for the special choice of a VARMA model.

Risk Management, Talks

RM/DID4856/000: **Risk management in financial and energy markets.**
Organiser: Walter Farkas (ETH Zürich, Switzerland)
Co-organiser: Juri Hinz (ETH Zürich, Switzerland)

Since 1998 ETH Zurich is hosting each year a Risk Day. The aim of the 2007 Risk Day, embedded as an Industry Day within ICIAM07, is to provide a forum for the discussion of new research and technical developments in risk management in financial and energy markets. The organizers have invited outstanding experts and practitioners to present and discuss the latest advances and new thinking in the fascinating area of risk management.
More information: http://www.math.ethz.ch/finance/Risk-Day-2007.html

Tests of covariance matrices. **Jens Wiedmann** (LGT Capital Management, Switzerland) RM/TID4858/x

How can it be decided, which kind of estimator of covariance matrices is more suitable to reflect the expected portfolio risk. A kind of Maximum-Likelihood-test is introduced for solving this problem. Some concrete test results concerning different bond portfolios are shown. For these bond portfolios the simple historic covariance matrix and covariance matrices of two-factor- and three-factor-models has been tested.

Risk-based capital models in life insurance. **Hans-Juergen Wolter** (Swiss Life, Switzerland) RM/TID4859/x

A number of recent initiatives such as the preparation for Solvency II for instance have led to an increase in the extent to which insurance companies manage their risk and capital. Until now, economic capital models have been developed by the best part of the global insurance industry; it is no longer the domain of the sophisticated insurance undertakings. And yet the design of economic capital models is still under way. The aim of this talk is to discuss the characteristics of proper capital models. Often, the requirements are controversial. A model that is impeccable from a conceptual point of view might be hard to implement. We conclude with some remarks on risk measurement, motivated by the fact that some European insurance regulators have begun to demand for multi-period risk measures.

Strategic risk management: ideas and questions. **Jörg Behrens** (Ernst and Young, Switzerland) RM/TID4860/x

While risk management is highly sophisticated and forms an integral part of the financial services industry, most firms still struggle to benefit from their analytical know-how when it comes to strategic planning. We discuss problems and ideas to bridge the gap between the two worlds.

RM/DID4856/000: **Risk management in financial and energy markets.** #2
Organiser: Hans-Jakob Luethi (ETH Zürich, Switzerland)
Co-organiser: Walter Farkas (ETH Zürich, Switzerland)
Co-organiser: Juri Hinz (ETH Zürich, Switzerland)

(For abstract, see session #1 above.)

Gas portfolio and transport optimization. **Alexander Boogert** (Essent Trading BV, The Netherlands) RM/TID4862/x

The transport of natural gas has received significant attention in the last months with the large price spikes in the UK facing sudden cold weather and the flow stop from Russia to Ukraine. Transport is a necessity in a world where gas sources are far removed from the gas demand, and in which a gas portfolio easily spans several countries. Meanwhile, the range of options within a gas portfolio is growing with an increasing number of instruments and increasing international gas trading. This has led to a situation where decisions have become non-trivial. The objective of this article is to describe the construction of an integrated approach for gas portfolio and transport optimization.

Investment models in restructured electricity markets subject to risk. **Yves Smeers** (Université Catholique de Louvain, Belgium) RM/TID4863/x

Capacity expansion optimization models dominated the area of investment in generation during the former days of the regulated electricity sector These models have lost some of their appeal today and other tools , some inspired by the theory of real options, have replaced them. We reconsider the old capacity expansion model that we expand into equilibrium models in a risky environment. For the sake of tractability and robustness we assume no market power. We first model risk by assuming firms with different cost of capital; this equilibrium model deviates minimally from the usual capacity expansion model (which assumes a single cost of capital). Alternatively we also consider that the risk attitude of firms is represented through risk functions; this forces one to consider a stochastic equilibrium model. We compare the approach to equilibrium (not optimization) models of the real option type.

Telecommunications, Plenary Talk

TC/IT4921: *Future challenges in mobile telecommunication industry*
Hartmut Kremling (Vodafone D2 GmbH, Germany)

Since the mobile telecommunication industry is suffering from saturated markets, customer's demands are rising. Market shares are allocated based on tariffs, network quality and the variety and quality of offered services. Therefore changes and innovations are omnipresent. Mobile operators are facing a variety of challenges in operating their existing networks and deploying future network technologies. On one hand convergent services, increasing bandwidth demand and significantly evolving traffic patterns due to new multimedia services require additional network resources and more complex network topologies. On the other hand, increasing cost pressure forces operators to streamline their network in order to allow for a more efficient design and operation. Thus optimisation methods become increasingly important to design, build and operate cost efficient networks and to cope with the expected customer demands for the future. Based on novel network standards and all IP, novel broadband services need to be invented in order to generate customer demands and service usage. Services like VoIP, IPTV, location-based and personalised services and advertising are the future. Increasing media consumption and mobile-internet convergence will be achieved by user-friendly communication portals and convergent multimedia services. Network and service innovations will only be successful, if increasing complexity and dimensionality are reduced by powerful algorithms for compression and customer profiling.

Telecommunications, Talks

TC/DID4906/015: **Optimization of telecommunication infrastructure.**
Organiser: Martin Grötschel (Zuse-Institut Berlin, Germany)

Optimization/equilibrium problems coming from regulation process in the mobile telecommunication industry. **Alejandro Jofré** (Universidad de Chile) TC/TID4917/015

Computing access charges in economic regulation process for a mobile telecommunication industry requires in many countries the optimal design of an efficient representative mobile telecommunication company providing communication services to satisfy the demand. For these companies the access charges usually represent an important percentage of their incomes. In this talk we show how the computation of the access charges requires optimization/equilibrium models connecting the demand, the optimal design of networks (antennas, switches) and financial computation aspects. We show then how the level of access charges affect the demand producing an iterative equilibrium process whose solution have an interesting economic meaning. This Optimization/equilibrium procedure is being currently used for a couple of regulators and it is particularly important for countries where the demand for mobile telecommunication services is strongly increasing.

Joint design and pricing on a network. **Martine Labbé** (Université Libre de Bruxelles, Belgium) TC/TID4918/015

In order to optimize revenue, service firms must integrate within their pricing policies the rational reaction of customers to their price schedules. In the telecommunication industry, this process is all the more complex due to interactions resulting from the structure of the supply network. In this paper, we consider a streamlined version of this situation where a firm's decision variables involve both prices and investments. We model this situation as a joint design and pricing problem which we formulate as a mixed-integer bilevel program, and whose properties are investigated. In particular, we take advantage of a feature of the model that allows the development of an algorithmic framework based on Lagrangean relaxation. This approach is entirely novel, and numerical results show that it is capable of solving problems of significant sizes.This is joint work with Luce Brotcorne, Patrice Marcotte, and Gilles Savard.

Network design with multi-period pricing: modelling and solution techniques with computations for the case of optical backbone networks. **Iraj Saniee** (Alcatel–Lucent Bell Laboratories, USA) TC/TID4919/015

We describe telecommunication network design models in which demand is an endogenous variable and affects and is affected by equilibrium prices of service and bandwidth. We assume that the network operator must make investment decisions over a multiperiod planning horizon while facing possible changes in technology, typically involving a steadily decreasing per-unit cost of capacity. In these talk we deviate from the traditional monopolistic models in which demand is given as an exogenous input parameter, and the objective is to minimize capacity deployment costs. Instead, we assume that the carrier sets end-to-end prices of service and bandwidth at each period of the planning horizon, which determine the demands that are to be met, using a plausible and explicit price-demand relationship. The resulting demands must then be routed, requiring an investment in capacity. The objective of the optimization is now to simultaneously select end-to-end prices of service and bandwidth and network installed capacities at each period of the planning horizon, so as to maximize the overall net present value of expanding and operating the network. The resulting optimization problems pose significant challenges to standard optimization techniques. The complexity of the model, its nonlinear nature, and the large size of realistic problem instances motivate the development of efficient and scalable solution techniques. We illustrate the modeling and solution techniques and approximations that we have used for the case of large-scale optical networks with protection requirements and compare and contrast with solutions derived from some existing non-linear optimization packages.Parts of this presentation are based on joint work with Daniel Bienstock, Olga Raskina and Qiong Wang.

Planning of optical core networks. **Joerg Eberspaecher** (TU München, Germany) TC/TID4920/015

Wavelength-division multiplexing (Wdm) technology in optical core networks enables very high bitrates and increased flexibility. To be prepared for new multimedia services and the increasing cost pressure network providers are forced to plan their networks carefully, not only before deployment, but also during the operation (online-planning). Network planning is a complex process that involves a number of subtasks which are typically strongly dependent on each other. The topological planning determines the location of switching nodes and where fiber links have to be provided. Based on this physical infrastructure and a given traffic matrix it is possible to perform the routing of demands. In order to be able to compensate for

network failures, it is essential to allow for alternative paths between the nodes. Hence, the physical network structure must be sufficiently meshed to allow for route diversity. Another routing aspect is the signal quality along the transmission path to guarantee a certain quality-of-service. The advent of transparent end-to-end transmission by optical signal switching at nodes poses additional requirements for transmission engineering since we have to take into account signal attenuation, dispersion, and nonlinear fiber effects.This talk gives an overview of optical core network planning. It presents typical modeling tasks of the design process and sketches the main methods currently applied in network planning. The typical design goal is to minimize total network costs in terms of investment costs (capital expenditures CAPEX) and also operational expenditures (OPEX). In order to provide optimal network configurations, mathematical programming is a well suited technique that is often applied to planning tasks. Depending on the network modeling, linear, integer linear as well as nonlinear programs can be used.However, the computational complexity and time critical issues such as online network configuration often require solutions based on fast heuristics. Generally, it is crucial to decompose the complex planning process into adequate subproblems that can be solved independently of each other. In the talk we present typical design problems, show solution examples and list a number of open issues which can best be tackled by joint efforts of network designers, system engineers, and scientists from mathematics.

TC/DID4906/015: Optimization of telecommunication infrastructure. #2

Organiser: Martin Grötschel (Zuse-Institut Berlin, Germany)

(For abstract, see session #1 above.)

Optimization of 2G/3G radio networks. **Andreas Eisenblätter** (Atesio GmbH, Germany) TC/TID4907/015

The development of wireless mobile communications over the past decade is breathtaking. So are the multi-billion Euro investments of radio network operators for establishing and maintaining high quality network infrastructure. Mathematical optimization has proven to be a very powerful instrument for designing cost efficient networks and for tuning network quality (prior to roll-out as well as during operations). This talk highlights impressing examples from projects with GSM and UMTS network operators. These success stories build on the ability to identify appropriate system models and on the availability of powerful mathematical optimization tools. They also illustrate the importance of close collaboration among radio engineering experts and mathematicians.

Efficient multi-carrier transmission: reflexive subspace of L_1 and Szemerédi's theorem on arithmetic progression. **Holger Boche** (Fraunhofer HHI Berlin, Germany) TC/TID4923/015

Multicarrier transmission is a very prominent transmission technique for wireless communication systems. The basic idea is to use the orthogonal Fourier system for the information transmission. One important problem in application of multicarrier transmission is to control the peak-to-power ratio; i.e., the L_1-norm of the transmission signal. One approach to solve the peak to average power reduction problem is to select a certain subset of the Fourier system for the information transmission and to use the complementary subset of the Fourier system for the peak to average power reduction. This is closely connected with the problem of characterizing the reflexive subspace of L_1. Szemerédi's theorem on arithmetic progression is used to analyse the properties of the chosen subset of the Fourier system for the information transmission.

Geometric routing in mobile ad hoc *networks.* **Francois Baccelli Baccelli** (École Normale Supérieure de Lyon, France) TC/TID4924/015

Geometric/geographic informations can be used to design new distributed multi-hop routing algorithms for mobile ad hoc wireless networks.In a first typical example, when a given packet is located at some tagged node, the next hop on the packet's route is chosen as the nearest among the nodes which are closer from the packet's destination than the tagged node. In a second typical example, one selects as next hop the node being the closest to the destination among the set of nodes which receive this packet successfully when broadcasted by the tagged node. Such algorithms can be used both in the point to point case and in the multicast case.The aim of this talk is to review a few analytical results which were recently obtained on such routing algorithms using stochastic geometry. Within this framework, random routes are built on realizations of homogeneous Poisson point processes of the Euclidean plane. The geometry of these routes can be analyzed thanks to the locality of next hop definition and the mean performance of the algorithms can then be characterized via averages computed over all Poisson configurations.

Optimization models and methods for designing wireless local-area networks. **Edoardo Amaldi** (Politecnico di Milano, Italy) TC/TID4922/015

Wireless Local Area Networks (WLANS) are becoming pervasive in working environments as well as public areas. Their rapid spread and increase in size call for quantitative methods to support decisions in designing high-performance WLANS. Considering as efficiency measure the sum over all users of the fraction of time they can access the network, the problem of deciding access points location and channels assignment so as to maximize network efficiency gives rise to challenging nonlinear variants of the set covering problem. We discuss mathematical programming models and methods to tackle versions of the problem, which capture important features of these networks, and we report some computational results.

Different parts of this presentation are joint work with S. Bosio, A. Capone, M. Cesana, F. Malucelli and D. Yuan.

Transport Systems, Talks

TR/DID1099/015: **Modelling and simulation of transport systems.**

Organiser: Michel Bierlaire (École Polytechnique Fédérale de Lausanne, Switzerland)

The complexity of transportation systems requires advanced mathematical models and algorithms to assist in their design, implementation and operations, as well as efficient and user-friendly pieces of software.

Although conceived and developed mainly in the academic community, advanced techniques have made their way to the industry, and are now distributed by various companies. These companies not only have contributed to the transfer of knowledge and technology to practionners, but are also active in research and developement.

The objective of this industry day is to present some of these companies, discuss the challenges associated with the use of advanced mathematical models in practice, and identify how industries and researchers from academia can better collaborate in the future.

Online microscopic traffic simulation to support real-time traffic management strategies. **Jaime Barcelo** (Universitat Politècnica de Catalunya, Spain) TR/TID4119/159

A timely response to incidents or other type of conflicting situations, recurrent or not, is a key requirement of any real time traffic management system, namely in large complex networks, but for a proper and improved performance of such system addtional functions are necessary: a decision making process assisting the trafic operator in identifying which could be the more appropriate management strategy to solse the identified problem; the capability of testing before implementation whether the selected strategy will have the expected impact or not and an anticipatory capability to forecast the short term evolution of traffic conditions to prevent the undesired effects of congestion. This paper presents the design and implementation of a system with these characteristics based on AIMSUN microscopic simulator and its application to some real life projects.

Optimisation algorithms for airline management . **Alberto De Min** (APM Technologies SA, Switzerland) TR/TID4573/159

APM Technologies SA is based in Geneva, Switzerland, and produces modular management software for airlines. APM products provide informed, intelligent solutions to problems related to aircraft scheduling, aircraft operations, aircraft maintenance, crew pairing, crew roster, disruption recovery and financial profitability. This talk reviews the mathematical approach followed by APM and describes the minimization algorithms implemented in its products.

A hybrid traffic-simulation model. **Andres Rabinowicz** (Caliper Corporation, USA) TR/TID4690/159

This paper describes a traffic model designed to simulate vehicles at varying levels of fidelity in an integrated hybrid modeling framework. Each of three model fidelities, including microscopic, mesoscopic, and macroscopic, is assigned to any chosen set of roadway segments, contiguous or dispersed, in a single network model and is used to simulate the movement of traffic through those segments. The microscopic model simulates individual vehicles based on a combination of sub models including car-following and lane changing. The mesoscopic model simulates vehicles as members of traffic cells and streams, their movements regulated by the density of the cell or stream of which they are a part based on speed-density relationships. Lastly, the macroscopic model uses volume-density relationships to estimate travel times, on which vehicle movements are based. The framework presented in this enables the simulation of very large networks in a way that makes the best use of available data and computing resources without having to partition the network or rely on disjoint models.

GAMM 2007 Embedded Meeting

01: Multi body dynamics (Mehrkörperdynamik)

02: Biomechanics (Biomechanik)

03: Damage and fracture (Schädigungs- und Bruchmechanik)

04: Structural mechanics (Strukturmechanik)

05: Oscillations (Schwingungen)

06: Material models in solids (Materialmodelle für Festkörper)

07: Coupled problems (Gekoppelte Probleme)

08: Multiscales and homogenization (Mehrskalen und Homogenisierung)

09: Turbulence and reactive flows (Turbulente und reagierende Strömungen)

10: Viscous flows (Reibungsbehaftete Strömungen)

11: Compressible flows (Kompressible Strömungen)

12: Waves and Acoustics (Wellen und Akustik)

13: Dynamics and Control (Dynamik und Regelung)

14: Flow Control (Magnetisch kontrollierte Strömungen, Strömungskontrolle)

GAMM, Plenary Lectures

GA/IT5030: Richard von Mises Prize Lecture II: *Explicit high-order one-step finite-volume and discontinuous Galerkin schemes on unstructured triangular and tetrahedral meshes for hyperbolic balance laws*
Michael Dumbser (Universität Stuttgart, Germany)

In this talk we present several building blocks for the construction of arbitrary high order accurate explicit one-step schemes in time for the solution of linear and nonlinear hyperbolic balance laws with stiff and non-stiff source terms on unstructured triangular and tetrahedral meshes in two and three space dimensions. The spatial discretization operator on unstructured meshes is either based on high order accurate WENO finite volume (FV) schemes or on a high order accurate discontinuous Galerkin (DG) approach.

The main feature of the proposed schemes is the particular time-discretization, which leads to explicit one-step methods in time that automatically match temporal accuracy with spatial accuracy. The explicit one-step nature of the schemes does not only allow for an efficient MPI parallelization on modern supercomputers, but also allows the easy implementation of time-accurate local time stepping for time-dependent problems, at least when using DG space operators. For hyperbolic systems with non-stiff source terms the element-local solution is expanded within one time step in a temporal Taylor series where then the classical Cauchy–Kovalewski procedure is used to replace time-derivatives with space derivatives using repeated differentiation of the original governing PDE. Unfortunately, in the case of stiff source terms, a temporal Taylor series expansion is no longer appropriate. Thus, a new element-local space-time DG method is used for time-discretization in order to predict the time-evolution within each element locally within the current time step. This new approach allows the construction of asymptotically consistent schemes for hyperbolic PDE with stiff source terms with any desired accuracy in space and time.

Using the WENO FV space discretization operators, we show numerical convergence results up to sixth order of accuracy in space and time for the compressible Euler equations of gas dynamics on triangular and tetrahedral meshes in two and three space dimensions. Furthermore, various unsteady two- and three-dimensional flow problems with smooth and discontinuous solutions are computed to validate the accuracy of the approach and to underline the non-oscillatory shock-capturing properties of the method. As an outlook to future applications, first results for the compressible unsteady Navier–Stokes equations on unstructured triangular meshes are shown. For hyperbolic systems with stiff source terms, convergence results and several test cases underlining the asymptotically consistent behaviour of the method are also presented.

Using the DG space operators, we show numerical convergence results and applications in three space dimensions using the proposed one-step time discretizations together with the new time-accurate local time stepping approach. Applications are shown for the linearized Euler equations commonly used in computational aeroacoustics (CAA), for the Maxwell equations and for the equations of linear elasticity in heterogeneous anelastic and anisotropic media as well as for linear elasticity in porous media, where the source terms in the governing PDE may become stiff in the low-frequency range.

GA/IT5031: Richard von Mises Prize Lecture I: *Model reduction of differential-algebraic equations*
Tatjana Stykel (TU Berlin, Germany)

Model order reduction play a significant role in simulation, control and optimization of large-scale differential–algebraic equations (DAEs) that arise in computational fluid dynamics, circuit simulation and multibody dynamics. The aim of model reduction is to approximate a large-scale dynamical system by a reduced-order model that captures the main features of the original system and has a small approximation error. In this talk we give an overview on model order reduction techniques for linear DAE systems and demonstrate their performance on practical problems.

GA/IT4717: *Quasi-continuum orbital-free density functional theory: a route to multi-million-atom electronic structure calculations*
Kaushik Bhattacharya (California Institute of Technology, USA)

This talk will describe a method for doing electronic structure calculations at macroscopic scales. Density functional theory, a formulation of quantum mechanics, has provided insights into various materials properties in the recent decade. However, the computational complexity of this approach has made other aspect, especially those involving defects, beyond reach. We describe a method that enables the study of a multi-million atom cluster using orbital free density functional theory with no spurious physics or restrictions on geometry. The key idea is a systematic means of adaptive coarse-graining retaining full resolution where it is necessary and coarsening where it is not with no patches, assumptions or structure. We demonstrate the method, its accuracy under modest computational cost and the physical insights it offers using various examples. Our calculations reveal that multi-million atom computational samples are inevitably required for predicting bulk properties of materials from orbital-free density-functional theory.

This talk is based on joint work with Vikram Gavini and Michael Ortiz.

GA/IT4571: *Tracking control of distributed-parameter systems: from theory to applications*
Andreas Kugi (TU Wien, Austria)

In this talk some recent results on the tracking control of distributed-parameter systems (DPS) are discussed and demonstrated by means of several application examples. Thereby, we utilize the so-called two-degrees-of-freedom control structure comprising a feedforward part for reference tracking and a feedback part for stabilizing the tracking error dynamics. Basically, there exist two approaches when dealing with the controller design for DPSs. First, in the so-called early lumping approach, the DPS is discretized w.r.t. the spatial coordinates and the controller design is based on the resulting system of

(nonlinear) ordinary differential equations. This often brings along rather complex control laws and does not take into account the distributed-parameter nature in a systematic way. In contrast to this, we focus on the so-called late lumping approach where the controller design relies on the DPS and the control law is then approximated for the purpose of real-time implementation.

In recent years there have been significant advances in extending the concepts of differential flatness and passivity-based as well as backstepping control, well established for (nonlinear) finite-dimensional systems, to the infinite-dimensional case. Clearly, in contrast to finite-dimensional systems there is no general approach which applies to the whole class of DPSs. Therefore, we focus on special examples each representing a certain class of DPSs. Among these examples we present the high-dynamic motion control of a piezoelectric cantilever, the control of a trolley carrying a heavy chain, the trajectory tracking of an (unstable) diffusion–convection–reaction system with nonlinear reaction rate and the temperature control in a steel-slab.

GA/IT4791: *On unsteady boundary-layer separation*
Anatoly Ruban (University of Manchester, UK)

The boundary-layer separation problem has been a focus of attention in fluid dynamics since 1904, when Prandtl introduced the notion of the boundary layer in high Reynolds number flows. In his seminal paper, Prandtl not only formulated the boundary-layer equations, but also gave physical explanation of the flow separation as being associated with the formation of flow reversal region inside the boundary layer. This concept lies in the foundation of all subsequent studies of the boundary-layer separation, including the theory of viscous–inviscid interaction. Also known as the triple-deck theory, it was formulated simultaneously by Neiland (1969) and Stewartson & Williams (1969) in application to self-induced separation in supersonic flows.

Later many researchers were involved in the development of the theory, and it became clear that the viscous–inviscid interaction governs the flow separation in wide variety of physical situations. However, summarising the results of a century long effort in this field, one has to admit that despite the significance of the progress made, many aspects of the theory of separated flows remain unresolved. Most notably, the theory remains predominantly restricted to two-dimensional, steady flows.

In this talk we shall discuss the separation of unsteady boundary layers, when alternative forms of separation become possible; these might not even involve the flow reversal. In the first part of the talk, the so called *collisional separation* will be considered. Theoretically it may be investigated based on discontinuous solutions of the boundary-layer equations. Such solution are encountered in various physical situations. We shall show that the discontinuities (by analogy with gas dynamics, we call them *pseudo-shocks*) are the centres of the fluid eruption from boundary layers.

In the second part of the talk, we shall discuss unsteady boundary-layer separation under the conditions when it may be treated (if considered in the coordinate frame moving with the separation point) as steady separation on a moving wall. Both cases of upstream and downstream moving wall will be studied. Interestingly enough, in the former case the flow separation requires a *favourable* pressure gradient to be imposed upon the boundary layer.

GA/IT4838: *Ferrofluids: magnetically controllable liquids*
Stefan Odenbach (TU Dresden, Germany)

Complex fluids with a flow behaviour differing significantly from the behaviour of normal liquids like water or oil exhibit numerous fascinating flow effects. This becomes especially interesting if the fluids properties and flows can be controlled by external forces.

Prominent examples for fluids allowing such an external control are suspensions of magnetic nanoparticles commonly known as ferrofluids. They exhibit normal liquid behaviour coupled with superparamagnetic properties leading to the possibility to control their flow and change their properties by means of moderate magnetic fields in the order of $10\,\mathrm{mT}$. With such fields, which can be produced easily with small electromagnets or by means of commercial permanent magnets, forces comparable to, for example the gravitational force, can be exhibited to ferrofluids. The comparably easy magnetic control gave rise to the development of numerous applications of ferrofluids in various technical and medical areas which partly gained importance in everyday life.

Within the talk the origin of the magnetic influence, its fluid mechanical consequences as well as the application possibilities in mechanics, medicine and other fields will be outlined and illustrated with a couple of experiments.

GA/IT4721: *Secret and joy of configurational mechanics: from foundations in continuum mechanics to applications in computational mechanics*
Paul Steinmann (TU Kaiserslautern, Germany)

Configurational mechanics has developed into a very active and successful topic both in continuum mechanics as well as in computational mechanics over the recent years. On the continuum mechanics side the basic idea is to consider energy variations that go along with changes of the material configuration. Configurational forces are then energetically dual to these configurational changes. Configurational forces take the interpretation as being the driving forces in the kinetics of defects; like e.g., cracks, inclusions, phase boundaries, dislocations and the like. On the computational side it turns out that a discretisation scheme brings in arteficial, discrete configurational forces that indicate in a certain sense the quality; e.g., of a finite-element mesh. This information can then be used in order to optimize the nodal material positions. Surprisingly, even driven by energetical arguments, it turns out that a finite element mesh optimized with respect to discrete configurational forces also renders superiour results in terms of classical error measures. The talk will span the field from the underlying theoretical foundations over the algorithmic challenges to various computational applications.

01, Short Communications

GA/CTS4896/01: **Materials, motion and stability.**

Organiser: Martin Arnold (Universität Halle–Wittenberg, Germany)
Co-organiser: Hartmut Bremer (Universität Linz, Austria)

Die Discrete Element Method (DEM) in der Geotechnik. **Eva Heesen** (TU Hamburg–Harburg, Germany), Edwin Kreuzer (TU Hamburg–Harburg, Germany) GA/CT2121/001

Hafenanlagen werden häufig auf schlechtem Baugrund gebaut und müssen daher auf Tausenden von großen Pfählen gegründet werden. Für die Planung von Hafenanlagen ist die Tragfähigkeit der Pfähle also von entscheidender Bedeutung. Derzeit können Pfahltragfähigkeiten aber nur im Nachhinein bestimmt werden. Die Schwierigkeiten in der Vorhersage entstehen durch die starken Veränderungen der Bodeneigenschaften während der Pfahlinstallation. Ergebnisse aus bodenmechanischen Voruntersuchungen haben nur noch wenig Aussagekraft. Bis heute ist ungeklärt, welche Bruch- und Verdrängungsmechanismen bei der Pfahlherstellung das Bodenverhalten bestimmen. Klassische bodenmechanische Ansätze versagen meist komplett. Die Modellierung des Pfahlrammens mit der Finiten Elemente Methode (FEM) wiederum ist problematisch, weil derzeitige Materialmodelle die Scherfugenbildung im Boden nur unzureichend abbilden können, Scherfugen aber eine entscheidende Rolle bei der Modellierung des Nahfeldes des Pfahls spielen. Daher wird gezeigt, wie die maßgeblichen Mechanismen bei der Pfahlinstallation sowie deren Einfluss auf das Tragverhalten des Pfahls mit Hilfe der Discrete Element Method (DEM) untersucht werden können. In der DEM wird der Boden als Granulat betrachtet, das aus einzelnen Partikeln besteht, die miteinander in Wechselwirkung stehen und sich gegeneinander verschieben können. Auf diese Weise können große Verschiebungen sowie Kornrotationen problemlos modelliert und somit kann auch das Nahfeld des Pfahls adäquat abgebildet werden. In dem hier verwendeten zweidimensionalen Modell werden die Partikel als konvexe unregelmäßige Polygone modelliert. Erste Ergebnisse der Pfahlmodellierung wie z.B. Verschiebungsfelder, Kornrotationen und Veränderungen der Lagerungsdichte werden in Abhängigkeit von Pfahlrauhigkeit und Eindringgeschwindigkeit vorgestellt.

Application of the discrete-element method to model cohesive materials. **Timo Gaugele** (Universität Stuttgart, Germany), Peter Eberhard (Universität Stuttgart, Germany) GA/CT2729/001

The discrete element method (DEM) has been widely used in the past to model granular materials like powder and sand. In recent years this approach was adopted by engineers in geomechanics and civil engineering to model geomaterials like concrete or marl. However, most modeled geomaterials exhibit very brittle behavior when loaded. Here, it is investigated if the so far used approach can be advanced to model materials that exhibit ductile behavior to some extent as well. Different models based on the DEM for the simulation of cohesive materials are presented. Starting from a basic two-dimensional non-cohesive model with circular particles the model is enhanced by including massless beam elements which represent particle bonds to introduce cohesive forces between adjacent particles. The particle bonds are represented by force laws and can sustain only a specified stress until failure. By implementing different force laws it is investigated if the composite made up of bonded discrete elements displays realistic elastic properties. As the bonds can only be loaded to a certain limit a failure criterion is used to detach and remove bonds. Once a bond is detached it can never be restored. By using different failure criteria it is to be investigated if the composite exhibits qualitatively correct failure modes.

Real-time simulation of quasi-static rod deformations. **Joachim Linn** (Fraunhofer ITWM, Kaiserslautern, Germany), Thomas Stephan (Fraunhofer ITWM, Kaiserslautern, Germany) GA/CT4063/001

We present a model of flexible rods, based on Kirchhoff's geometrically exact theory, which is suitable for the fast simulation of quasi-static deformations within VR (vitual reality) or FDMU (functional digital mock up) applications. Unlike simple models of *mass & spring*-type typically used in these application areas, our model provides a proper coupling of bending and torsion. The computational approach comprises a variational formulation combined with a finite-difference discretization of the continuum model. Approximate solutions of the equilibrium equations for sequentially-varying boundary conditions are obtained by means of *energy minimization* using a nonlinear CG method. The computational performance of our model proves to be sufficient for the interactive manipulation of flexible cables in assembly simulation. A *dynamical* version of our model, which accounts for inertial effects, can also be integrated into MBS environments to provide a fast simulation of flexible rod-like structures.

On stability problems of the space elevator. **Michael Schwarzbart** (TU Wien, Austria) GA/CT2366/001

We investigate the stabilty of steady-state motions of an extremely long cable in circular orbit around the Earth. Possible applications of such a cable are to use it as track of an Earth to space elevator or to lift payloads with the cable rotating in its orbital plane. These are also two typical examples for a classification of synchronous and non-synchronous ([1]) motions of the cable. We consider both cases and formulate, first, the stability problem of the motion of an anchored synchronous cable for small motions of the pivot point, which might be necessary to avoid a collision with a low orbit spacecraft. Secondly, we study also the stability of the motion of a nonsynchronous rotating cable ([1]) with a length of the order of 1/3 of the diameter of the Earth. The realisation of these elevator concepts became feasible technologically at about 1990 when a new high strength and low weight material, called carbon nanotubes, was discovered. For our numerical calculations we assume defective carbon nanotubes with more realistic technical material properties ([2]).

[1] Moravec Hans, 1977, *A Non-Synchronous Orbital Skyhook.* The Journal of the Astronautical Sciences, Vol. XXV, No. 4, pp. 307-322.
[2] Pugno Nicola, Schwarzbart Michael, Steindl Alois, Troger Hans, 2006, *On the stability of the track of the space elevator.* Paper No. IAC-06-D4.2.05, IAF-Congress Valencia 2006

A holistic finite-element and multi-body-systems approach for the virtual product development. **Corinna Barthel** (Universität Magdeburg, Germany) GA/CT4078/001

The enhancement and application of a holistic virtual product development process is one of today's main research and development activities in engineering due to the expected reduction of time and costs and the improvement of the product quality.

The paper first presents the results of an automated generation of adaptive mechanical models, including the derivation of qualified submodels and their integration into a holistic model. The focus is on the application of a multi-body systems (MBS) approach in connection with finite element analysis (FEA) and control.

In general the modelling starts with CAD-based geometry data which have to be extended by parameters determining the physical and functional behaviour of a system. In dependence of the specific tasks to be solved, different types of models can be derived, such as a precise local model, if the local stresses distribution is required or a rough overall model, if the trajectory of the motion of a mechanical system is in the focus of the investigation. The type of model, which is created by the engineer, significantly affects the quality of the results. Consequently, this process should be automated to a possible extent and controlled by error estimates.

In the paper it is shown, that a combination of a multi-body systems approach including different elastic finite element models as well as multi-field sub-models and also control results in a sufficiently accurate model designed for solving a large variety of engineering problems. The presentation and verification of the results in a virtual reality environment show the advantages of such approach for an effective product development process.

The numerical analysis of the trapezoidal thread rolling process . **Maciej Kukielka** (Koszalin University of Technology, Poland), Leon Kukielka (Koszalin University of Technology, Poland) GA/CT2727/001

The thread rolling is difficult technological process. Improve quality and contemporary reduce manufacture cost of the trapezoidal thread expect knew of physical phenomena observed in the contact zone between rolls and deform workpieces. Therefore, this paper presents the physical and mathematical models of deformations (displacements and strains) and stress in the cold process of trapezoidal thread rolling. The process is considered as a geometrical and physical nonlinear, initial as well as boundary value problem. The phenomena on a typical incremental step were described using a step-by-step incremental procedure, with an updated Lagrangian formulation. The state of strains was described by Green-LagrangeŠs tensor, while the state of stress by the second symmetrical Pioli-KirchhoffŠs tensor. The object was treated as an elastic (in the reversible zone) and visco-plastic body (in non-reversible zone) with mixed hardening. The variational equation of motion in three dimensions for this case was proposed. Then, the finite elements methods (FEM) and dynamic explicit method (DEM) were used to obtain the solution. The application developed for the method of finite elements ANSYS, which provides a complex time analysis for displacement, strains and stresses occurring in the object. The recommendations concern modeling the trapezoidal thread rolling process, where reduce degrees of freedom in numerical model is very important and provide convergence calculated results for maximum stress and strain values in the thread surface layer, were elaborate. The influence a various process conditions on the states deformation and stress for examples calculations, were presented.

GA/CTS4893/01: Vehicle dynamics.

Organiser: Peter Eberhard (Universität Stuttgart, Germany)
Co-organiser: Martin Arnold (Universität Halle-Wittenberg, Germany)
Co-organiser: Hartmut Bremer (Universität Linz, Austria)

Recent developments in flexible multibody dynamics. **Andreas Heckmann** (DLR Aerospace, Germany), Ingo Kaiser (DLR Aerospace, Germany), Matthias Reiner (DLR Aerospace, Germany) GA/CT1704/001

In present days new technologies emerge and the demands on technical systems increase. Environmental issues such as noise gain more and more importance and the complexity of products is perpetually enlarged so that more technical domains are involved in the design process. These facts give reason to extend the modelling capabilities in flexible multibody dynamics concerning three different issues, namely (i) the consideration of thermoelastic behaviour, (ii) the dynamic rotor analysis for vibroacoustic post-processing and (iii) the acasual, symbolic modelling of flexible bodies for heterogeneous technical systems. All these extensions are aligned with the goal to incorporate the analysis of flexible bodies in a design process with many different demands and needs.

(i) Mechanical processes are often associated with heat generation due to friction or energy transformation. E.g. in friction brakes the heat generation is even at the core of the process and may feed back on the mechanical behaviour. With this background, the proposed modal multifield approach provides an efficient way to consider the thermoelastic properties of flexible bodies.

(ii) According to the so-called arbitrary Lagrangian-Eulerian (ALE) representation of flexible bodies, the motion of an elastic rotor may be decomposed in a specific way, so the reference frame is neither fixed in space nor connected with material particles. This approach has been found to be adequate for rolling contact problems such as a railway wheelset on rails and enables the straight-forward consideration of the gross angular motion of a wheelset for the numerical evaluation of its sound radiation.

(iii) The object-oriented, high-level modelling language Modelica, developed by the non-profit Modelica Association provides a platform to incorporate multiple modelling domains such as hydraulics, pneumatics, mechanics, electric systems etc. in one common simulation environment. In the meantime this concept is additionally substantiated by a large set of ready-to-use component libraries including the new Modelica flexible bodies library. In the course of the talk the advantages of the symbolic, acasual modelling approach of Modelica for the design of technical systems with elastic bodies will be discussed.

Modellbasierte Optimierung aktiver Radaufhängungen. **Werner Schiehlen** (Universität Stuttgart, Germany) GA/CT1368/001

Beim Entwurf von Radaufhaengungen fuer Kraftfahrzeuge haben sich Mehrkoerpermodelle, welche durch die zufaelligen Strassenunbenheiten stochastisch erregt werden, bewaehrt. Zur Berechnung der Schwingungsantwort des Fahrzeugs stehen die numerische Simulation, die Spektraldichteanalyse und die Kovarianzanaylse zur Verfuegung. Zur Beurteilung von Aufhaengungssystemen werden die Varianzen der Aufbaubeschleunigung, der dynamischen Radlasten und des Arbeitsraumes der Radbewegung benoetigt, um Fahrkomfort und Fahrsicherheit zu bewerten.

Die Kovarianzmethode wurde fuer passive Radaufhängungen erfolgreich angewandt. Heute stehen jedoch die aktiv geregelten Radaufhaengungen im Mittelpunkt des Interesses, wobei die regelungstechnischen Methoden des Zustandsraums und des Frequenzgangs eingesetzt werden ohne die Varianzen zu beruecksichtigen.

In diesem Beitrag wird die Kovarianzanalyse auf aktive Radaufaengungen erweitert mit "Skyhook" Daempfern und aktiven Federn. Das Ergebnis zeigt den Einfluss der mechanischen Einwurfsvariablen Masse, Steifigkeit und Daempfung sowie der Reglerverstaerkungen auf. Damit laesst sich die Parameterempfindlichkeit der Entwurfsvariablen betimmen.

An optimal control algorithm for an autonomously driving car. **Matthias Gerdts** (University of Birmingham, UK) GA/CT2706/001

The driver of an automobile can be modeled by formulating a suitable optimal control problem. However, if the length of the drive is very long or if the course has a very complicated structure, the numerical solution of the optimal control problem becomes very difficult. Therefore a moving horizon technique is employed, where the global optimal control problem is splitted into a sequence of local optimal control problems which are combined by suitable continuity conditions.

We will report our experiences with this algorithm as it has been integrated in an existing car and allows to compute time optimal solutions for various handling courses in a robust way. The algorithm can be used for testing different setups of cars under the same conditions as the influence of a real driver is excluded.

Work-space analysis and maximal-force calculation of a face-shovel excavator using kinematical transformers. **Francisco Geu Flores** (Universität Duisburg–Essen, Germany), Andres Kecskemethy (Universität Duisburg–Essen, Germany), Alois Pöttker (Terex GmbH, Germany) GA/CT2374/001

This paper describes a method for the efficient determination of maximally allowed shovel forces for a heavy-load face-shovel excavator through its workspace. The method is based on the concept of “kinematical transformers”. In this concept, each multibody loop is regarded as a transmission element coupled by linear equations with the other multibody loops, allowing an efficient detection of closed-form kinematical solutions. Additionally, the method uses a graphical optimization approach to find the maximal digging forces for given positions of the shovel. An application-specific code has been realized using a combination of the object-oriented multibody library Mobile and symbolical equations. The method is applied to existing heavy-load excavators, showing that the computational effort can be reduced by a factor of more than 200 as compared to general purpose numerical codes.

Hybrid neural-network shock-absorber model. **Vladislav Pracný** (Universität der Bundeswehr Hamburg, Germany) GA/CT1088/001

Shock absorber is one of the main components of car’s suspension and its function is to control chassis movement. By turning the mechanical energy into heat unwanted vibrations are eliminated. As we know, the inner design of shock absorber is relativ complex, whereby the damping force is specified by the flow of damping oil through various valve assemblies. Further the temperature dependent viscos properties of damping oil, friction effects and the gas charge are effecting the damping force. The spline approach is not suitable, if all this phenomena have to be considered. Even though the spline function is widely applied in the full vehicle simulation. The principle advantages are its simplicity and optional changes of the characteristics, if e.g. influence of the shock absorber to the behaviour of the vehicle is investigated. A fairly modern approach is the neural network modelling based on the mathematical approximation of measured data. In this case, the components behaviour is described by an algebraic equation, where the information about the system is carried by a set of parameters, in general, with no physical meaning. If the parameters of the neural network are set properly, the approximation accuracy is very high. The main drawback of is the missing interpretability. To obtain accurate force prediction together with a system variability, spline and neural network approach are combined. Two forces in parallel $F_d = F_{spl} + F_{nn}$ are representing the damping force. The main velocity dependent shock absorber characteristics F_{spl} is determined by a spline function. By the neural network only the remainder force F_{nn} between measurement and spline approximation is represented. The neural network is defined as a function of immediate time history of velocity, actual displacement and actual temperature. Additionally to the force components a differential equation for the temperature evolution is defined. The hybrid shock absorber is implemented into a full vehicle model in ADAMS/Car and the influence to the vertical vehicle dynamics is investigated. The reference is a standard spline model.

GA/CTS4895/01: Modelling and integration techniques.

Organiser: Matthias Gerdts (University of Birmingham, UK)
Co-organiser: Martin Arnold (Universität Halle–Wittenberg, Germany)
Co-organiser: Hartmut Bremer (Universität Linz, Austria)

Numerical integration of multi-body dynamics employing control constraints. **Mahmud Quasem** (Universität Siegen, Germany), Peter Betsch (Universität Siegen, Germany), Stefan Uhlar (Universität Siegen, Germany) GA/CT3341/001

The present work deals with the control of underactuated multibody systems. Our approach is based on the use of servo (or control) constraints (see, for example, [1]) which are incorporated into the underlying rotationless formulation of multibody dynamics [2]. In this connection we focus on the stable numerical integration of the resulting set of differential-algebraic equations. In particular, we aim at an energy-consistent integrator which facilitates the algorithmic conservation of angular (and linear) momentum.

References

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Energy-momentum conserving integration of parallel manipulators. **Stefan Uhlar** (Universität Siegen, Germany), Peter Betsch (Universität Siegen, Germany) GA/CT2405/001

In the framework of a rotationless formulation for multibody systems, we present an investigation of spatial multibody mechanisms. The benefit of this kind of formulation is the design of energy-momentum conserving integration schemes, which facilitate a stable numerical integration of differential algebraic equations governing the motion for open-loop and closed-loop systems.

We introduce a coordinate augmenation technique for the incorporation of rotational degrees of freedom and subsequently perform a size-reduction to lower the computational costs and to improve numerical conditioning. In this connection a new approach to the systematic design of discrete null space matri-

ces for closed-loop systems is presented [1]. Furthermore the treatment of nonholonomic constraints is addressed.

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[1] P. Betsch, S. Uhlar Energy-momentum conserving integration of multibody dynamics, submitted for publication in Multibody System Dynamics.

A nonlinear finite-element framework for flexible multibody dynamics. **Nicolas Sänger** (Universität Siegen, Germany), Peter Betsch (Universität Siegen, Germany) GA/CT2457/001

We present a uniform treatment of rigid-body dynamics and nonlinear structural dynamics. The advocated approach is based on a rotationless formulation of rigid bodies, nonlinear beams and shells. In this connection, the specific kinematic assumptions are taken into account by the explicit incorporation of holonomic constraints. This approach facilitates the straightforward extension to flexible multibody dynamics by including additional constraints due to the interconnection of rigid and flexible bodies. We further address the design of energy-momentum schemes for the stable numerical integration of the underlying finite-dimensional Hamiltonian systems.

To demonstrate the superior numerical performance of the proposed methodology, the numerical examples deal with closed-loop multibody systems containing both rigid and flexible bodies undergoing large deformations.

Symbolic simplification of equations of multibody dynamics in VSD software. **Dmitry Vlasenko** (Universität Magdeburg, Germany), Roland Kasper (Universität Magdeburg, Germany) GA/CT3031/001

This paper introduces a new preprocessing method for the symbolic simplification of equations of motion of mechanical systems. The integration of the method in the component-oriented simulation tool VSD (Virtual System Designer) greatly improves the numerical efficiency of the software.

Due to the fact that the simulation of multibodies in VSD is performed in a strictly component-oriented way, mechanical submodels can be modelled, tested and compiled independently from each other. The tool is based on a non-iterative algorithm that is applicable to mechanisms with any joint type and any topology, including branches and kinematic loops. The simulation of big good-partitioned systems has complexity O(N), where N is the total number of simulating bodies.

The most time-expensive routines of the simulation process in VSD are the calculation of accelerations and the post-stabilization of constraints, which need the finding of roots of matrix equations. Accounting the sparsity of matrices the routineŠs numerical efficiency can be significantly improved. That is why we developed a preprocessing module in Maple software which performs the symbolic simplification of the QR decomposition and the complete orthogonal decomposition of matrices.

The use of the preprocessing module has the following advantages:

1. Sparse structure of matrices is used completely without any run time overhead.

2. The numerical operations with numerical elements of matrices are performed already during the translation.

3. Additional operations with arrays of indexes (like in usual sparse solvers) are not needed.

Tests show that the integration of the preprocessing module in VSD significantly reduces the computation cost of the simulation of multibodies.

A quasi-static approach for constrained systems in real-time simulation. **Bernhard Burgermeister** (Universität Halle–Wittenberg, Germany) GA/CT3551/001

The rapidly increasing complexity of multi-body system models in applications like vehicle dynamics, robotics and biomechanics requires qualitative new solution methods to slash computing times for the dynamical simulation.

Detailed multi-body systems are designed for accurate off-line simulation. For real-time applications simplified models are used. The presented quasi-static solution method focuses on accelerated computation of the low frequency parts of the solution of the nonlinear equations of motion. The high frequency parts are eliminated by neglecting some of the inertia forces and torques. This reduces numerical stiffness and allows larger step-sizes for the time-integration.

The efficient and real-time capable combination with existing highly efficient algorithms for multi-body dynamics ($\mathcal{O}(N)$ multi-body formalisms) requires appropriate integration methods that are adapted to the special structure of the multi-body formalism and solve the non-linear constraints with a small, limited number of calculation steps.

Work done in collaboration with M. Arnold (Martin–Luther–University Halle–Wittenberg, Germany) and A. Eichberger (INTEC GmbH, Wessling, Germany)

Simulation of constrained mechanical systems. **Panagiotis Koutsovasilis** (TU Dresden, Germany), Michael Beitelschmidt (TU Dresden, Germany) GA/CT3470/001

Motion equations of dynamic constrained mechanical multibody systems (MBS) are described by differential and algebraic equations (DAE). Various methods for simulating DAEs using commercial DAE-solvers are implemented. A comparison study concerning the quality of their results is presented. Issues, such as the importance of DAE-index, finding a consistent set of initial conditions, the drift-off phenomenon as well as the application of projection and stabilization techniques are discussed.

Keywords: DAE, constrained mechanical systems, index, comparison study.

GA/CTS4892/01: Friction, sliding, stiction.

Organiser: Christoph Glocker (ETH Zürich, Switzerland)
Co-organiser: Martin Arnold (Universität Halle–Wittenberg, Germany)
Co-organiser: Hartmut Bremer (Universität Linz, Austria)

To the rolling contact in multibody-systems. **Felix Fritz** (Universität Karlsruhe, Germany), Wolfgang Seemann (Universität Karlsruhe, Germany), Daniel Wilde (Universität Karlsruhe, Germany) GA/CT1192/001

Rolling motion in multibody-systems is often described by pure rolling with holonomic constraints. For a realistic motion however, it is necessary to know in which way lubrication and friction affect the rolling. Particularly due to lubrication, motion may change from pure rolling to sliding.

For the simulation of multibody dynamics, reduced models for contact stress and resulting forces are of interest. Therefore different models for normal and tangential forces in lubricated

rolling contact were examined. Due to limited simulation time general contact formulations could not be applied. Therefore specific contact models for rolling geometries (for example balls) have been implemented into Fortran environment.

A multi-body system with two-dimensional contact interface. **Stamm Wolfgang** (LuK GmbH & Co. oHG, Germany) GA/CT3130/001

In the present talk we introduce a multi body system of rigid bodies with 2D frictional surface-to-surface contacts. The problem of multiple contacts between rigid bodies is addressed within a regularization approach derived from the classic PRANDTL and REUSS model of time-independent plasticity. Analogous to common practice in continuum mechanics, discretization is done for the two-dimensional contact interface. The model incorporates sliding and sticking states of the contact. Friction properties, such as Stribeck curves, can be represented locally in this framework.

The proposed method is suitable for mechanical systems which can be treated as rigid bodies but need to include motions caused by the distribution of frictional forces in the contact region. As a technical example, investigations of a vehicle's clutch system are presented. The self-centering effect of two rotating disks contacting each other with a misalignment is examined.

Straight chain of interconnected mass points under the action of non-symmetric dry friction. **Igor Zeidis** (TU Ilmenau, Germany), Klaus Zimmermann (TU Ilmenau, Germany), Mikhail Pivovarov (TU Ilmenau, Germany) GA/CT1899/001

In [1], the motion of a linear oscillator under the action of a small non-symmetric Coulomb dry friction force is discussed. Here, we consider the motion of a chain of n interconnected equal material points with masses m placed on a rough straight line and connected by equal kinematical constraints $l(t)$. It is supposed that the system undergoes a small non-symmetric Coulomb dry frictional force $\varepsilon m F(\dot{x})$, $\varepsilon \ll 1$ acting from the surface contact with the ground on each mass point and opposite to the direction of motion. The magnitude of this force also depends on the direction of motion: $F(\dot{x}) = F_+$, if $\dot{x} > 0$, $F(\dot{x}) = F_-$, if $\dot{x} < 0$, $F(\dot{x}) = F_0$, if $\dot{x} = 0$, $-F_- < F_0 < F_+$, $F_- \geq F_+ \geq 0$. An averaging procedure is applied to the equation of motion. For $n \leq 5$ an explicit expression for the stationary "on the average" velocity V of the motion of the system as a single whole is found. For $n > 5$ an algebraic equation for the corresponding stationary velocity of the motion of the system is obtained. A dependence of stationary velocity on the number of mass points n in a chain and value of asymmetry $\mu = F_+/F_-$ is found. It is shown that the magnitude of the velocity of the chain increases with the increasing number of mass points n. This dependence is monotonous individually for even and not-even n. The obtained theoretical results can be used for the design of worm-like vibration robots.

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Stability analysis of the linear non-conservative systems with fractional damping. **Vladimir Kobelev** (Universität Siegen, Germany) GA/CT1409/001

In considering design problems for non-conservative systems the integral structural characteristics as fundamental frequencies, critical loads for instability and the sensitivity analysis plays an important part. In this lecture, the influence of small perturbation on a linear, non-conservative dynamical system exhibiting a flutter type bifurcation has been investigated. The methods for dynamical instability are applied to study the eigenvalue problem for governing equations with fractional derivatives, i.e. for a special class of pseudodifferential equations. The hereditary damping is described by means of fractional derivatives. To study the dynamical instability for non-conservative governing equations with fractional damping the method of auxiliary eigenvalue problem is applied. The stability conditions of generalized Lyapunov type for the system with hereditary damping were derived. Because the solution of damped one degree of freedom oscillator could not be represented in terms of exponent functions, the stability conditions for non-conservative systems with fractional damping are essentially of generalized Lyapunov type. Namely, the solution of the fractionally damped oscillator deliver two-parametrical Mittag-Leffler functions. The behaviour of Mittag-Leffler functions is similar to those of the trigonometrical functions of complex argument; thus, the vibration of fractionally damped oscillator is somewhat analogous to the vibration of common viscous oscillator by small damping. The modal decomposition of fractionally damped system with several degrees of freedom allows to establish the stability conditions in terms of the eigenvalues of the generalized eigenvalue problem.

The numerical analysis of the influence of the blankholder force and the friction coefficient on the value of the drawing force. **Paweł Kałduński** (Koszalin University of Technology, Poland), Leon Kukielka (Koszalin University of Technology, Poland) GA/CT3081/001

On this paper the numerical analysis of the drawing process with the blankholder is presented. The influence of the value of the blankholder force on the value of the drawing force is examined. A different friction coefficients of the sheet metal for die and blankholder is considered. A defect at the lack of the blankholder is presented. The analysis in the system LS-DYNA is passed. The material model with the consolidation power, isotropic and isothermal is used. Technological parameters of the sheet-metal to drawing, the die, the stamp and the blankholder from the literatures are chosen. Sample results of computer simulations with stress distributions in a disk is presented.

The numerical analysis and experimental research of influence of triangular Asperity's outline deviations, after turning on the burnished product's technological quality. **Agnieszka Kulakowska** (Koszalin University of Technology, Poland), Leon Kukielka (Koszalin University of Technology, Poland) GA/CT2733/001

The paper concerns determination dependence of preparing inaccuracy surface texture after previous treatment on the state and properties of burnished article's surface layer (SL). The researches were realized in two stages, in the first one numerical analyses were made, and in the second one experimental verification of receiving results. The application in ANSYS was elaborated. It makes possible to analyze the influence of outline deviations triangular asperity after turning on the surface roughness, the state of strains and stresses in SL after burnishing rolling. The variables in calculations are: height deviation of triangular asperity after turning $\Delta h_t = 0.01 \div 0.04$[mm], and its spacing deviation $\Delta s_t = 0.05 \div 0.2$[mm] as well as the depth of burnishing $g = 0.03 \div 0.39$[mm]. The calculations for the case of burnishing the triangular asperities with vertical angle $\theta = 120°$, from steel45 were introduced as an example. The simulation's results were used to elaborate the one parameter functions of regress. The essential influence of asperity's outline deviations after turning on the technological quality of burnished product was showed. The numerical analyses results were experimental verified. There were turned the regular asperities with triangular outline on the surfaces of cylindrical samples from steel45. The samples were characterizing

by the variable height deviation of neighboring asperities in range $\Delta h_t = 0 \div 0.05$ [mm]. Next the samples were burnished and the measurements of parameters of roughness R_a, R_z, R_t, $R_s m$ and Wt were executed. The one parameter graph of dependence of height's deviation after burnishing from height's deviation of asperity after turning, for three depths of burnishing, was prepared. The results of experimental researches and numerical analyses cover in 5% confidence interval.

GA/CTS4894/01: Robotics.

Organiser: Werner Schiehlen (Universität Stuttgart, Germany)
Co-organiser: Martin Arnold (Universität Halle–Wittenberg, Germany)
Co-organiser: Hartmut Bremer (Universität Linz, Austria)

Anwendung eines Schmerzsensors. **Frank Schiefer** (TU Braunschweig, Germany), Georg Ostermeyer (TU Braunschweig, Germany) GA/CT1523/001

Die Erforschung von Schmerz aus technischer Sicht ist ein bisher wenig behandeltes Forschungsgebiet. Ein erster Ansatz zur Problembeschreibung ist in [1] gegeben.
Die weitere Grundlage zur Anwendung eines Schmerzsensors ist ein Sensorkonzept zur Schmerzdetektierung [2,3], mit dessen Hilfe ein Energieeintrag gemessen wird, der als ein Schmerzmaß für technische Systeme infolge periodischer und stoß artiger mechanischer Beanspruchungen interpretiert werden kann. Dieses entwickelte Schmerzmaß enthält implizit u. a. frequenzselektive Informationen über das Zeitverhalten des Energieeintrages sowie über die Ruckbeanspruchung dynamischer Systeme.
Anhand eines einfachen Demonstrators, der beispielsweise ein Gehmaschinenbein oder einen Roboterarm darstellt, wird gezeigt, wie die Bahnplanung einer Bewegung hinsichtlich des Schmerzmaßes optimiert werden kann. Die so entwickelte schmerzoptimale Bahn wird darüber hinaus mit weiteren Optimalitäts-
kriterien der Bahnplanung verglichen. Im einzelnen werden schmerzoptimale Bahnen des Demonstrators beispielsweise mit weg-, zeit- und energieoptimalen Bahnen verglichen.

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[3] Ostermeyer, G.-P., Schiefer, F.: On Pain Detection in Multibody Systems, to appear in Applied Mechanics and Materials

Real-time FEM for haptic applications under consideration of human perception. **Gerhard Schillhuber** (TU München, Germany), Heinz Ulbrich (TU München, Germany) GA/CT2282/001

This work addresses the fast computation of contact forces for haptic applications using the finite element method. In general, a human operator interactively manipulates an object with a haptic input device. With the provided force feedback it is possible to display the occurring contact forces to the human operator. Typical applications include haptic simulations such as surgery simulators, robotics and force prediction in telepresence scenarios. To guarantee a realistic force feedback, accurate models need to be generated. The objects are modeled using the finite element method (FEM), such that deformable bodies can be taken into account. The drawback of a fine discretization is the high computation time for a certain contact and deformation state. In contrast, the FEM computation has to be performed within a several milliseconds to provide a continuous force feedback signal to the human. An analysis of the human perception of continuous force signals is presented. The results are integrated in a new iterative solution method for the FEM problem. Considering human perception reduces the number of evaluations, because the force changes, which are undetectable by the human, do not have to be computed. The dynamics of the multibody system are evaluated by using a time integration method. So various physical effects can be treated such as soft contact, friction and inertia. Simulation results are presented to show the capacity of the algorithm.

Continuous workspace analysis for parallel cable-driven Stewart–Gough platforms. **Tobias Bruckmann** (Universität Duisburg–Essen, Germany), Dieter Schramm (Universität Duisburg-Essen, Germany), Manfred Hiller (Universität Duisburg–Essen, Germany) GA/CT1834/001

Parallel cable-driven Stewart–Gough platforms consist of a movable end-effector which is connected to a machine frame by motor driven cables. Since cables can transmit only tension forces, at least $m = n + 1$ cables are needed to tense a system having N degrees-of-freedom. This results in a kinematical redundancy and gives $m - n$ degrees-of-freedom in the cable force distribution.

For this reason, the workspace analysis is complex and very time-consuming. Therefore, reliable and robust algorithms are demanded to calculate the resulting workspace for a given parameter set (cable winch positions and platform connection points). To analyze the workspace, discrete methods are widely used. However, the drawback of these methods is that intermediate points on the discrete calculation grids are neglected. Especially for parallel mechanisms, this may lead to false results and thus be dangerous. A promising way to avoid this kind of discretization problems may be by analyzing the workspace by so-called interval arithmetics. This contribution provides the basic ideas of a continuous workspace analysis for cable-driven Stewart-Gough platforms. The results of the interval analysis are illustrated for some geometric parameter sets. Noteworthy, the presented algorithms yield guaranteed workspaces and are usable for both the completely restrained systems ($m = n + 1$) as well as for the more difficult redundantly restrained systems ($m > n + 1$).

For practical application (e.g., in robotics), parameter synthesis to generate particular workspace geometries is mandatory. However, in general the resulting workspace gemomtries are very complex and not intuitive to the design engineer. Here, the extension of the analysis methods to methods usable for the synthesis is shown and presented along with an illustrative example.

New development of parallel robots and micro-robots with three, four and five degrees of freedom. **Doina Liana Pisla** (Universitatea Tehnicã Cluj-Napoca, Romania), Anneline Vidrean (Technical University Cluj-Napoca, Romania), Nicolae Plitea (Universitatea Tehnicã Cluj-Napoca, Romania), Adrian Pisla (Technical University Cluj-Napoca, Romania), Calin Vaida (Universitatea Tehnicã Cluj-Napoca, Romania) GA/CT2968/001

All over the world it can be noticed that the product miniaturisation is a central theme in product development for different application areas.

In robotics scientific research one of the most important approaches is concerning the raise of the positioning accuracy by the use of parallel structures. The progress of the industrial production, especially the development of the industrial robotics is more and more based on a new generation of robots

based on closed kinematic chains mechanisms, the parallel robots.

The parallel kinematic structures have a series of advantages that makes them proper for micro-robots building: the actuators positioned on the seating, actuators separation from the workspace, miniaturization capabilities, stiffness, high positioning precision and repeatability.

In the paper are presented some variants of parallel robots and micro-robots with three, four and five degrees of freedom, which are used for manipulation within the high precision assembling processes. For the parallel micro-robots were developed the geometric virtual models by using the Solid Edge virtual modeling software packages. The modeled solutions are developed with classical joints and with pseudo-elastic joints.

The corresponding kinematic models have been developed from some geometric models.

Experiments in non-smooth mechanics with a passive-actuated robotic arm. **Tobias Welge-Lüssen** (ETH Zürich, Switzerland), Christoph Glocker (ETH Zürich, Switzerland) GA/CT3039/001

Since every technical system has to deal with friction and impacts (e.g., bedstops due to a limited workspace) the motivation for examining such systems as non-smooth systems on a theoretical level is quite high. The proposed non-smooth mechanical system consists of a passive-actuated robotic arm, which has the shape of a 2-link serial manipulator and will be used as an experimental platform for the verification of control strategies for non-smooth mechanical systems.

In order to describe the different aspects of the model and the experimental behavior of the passive-actuated manipulator, the overall model and the result of various experiments performed on it will be presented.

The model takes the non-smooth behavior of the dynamics due to impacts and friction into account and incorporates the flexible properties of the physical structure, especially of both arms and of the shafts within the joints connecting two arms. In addition the electrically powered elements (motor respectively brake) and the measuring devices are included in the model.

Besides experiments for the identification of the system-parameters and the validation of the measuring devices, results for open-loop paths of precalculated time optimal trajectories will be shown and compared to the results based on a time-stepping simulation of the system.

A modified reliable distance algorithm for octree-encoded objects. **Cornelius Grimm** (Universität Duisburg-Essen, Germany), Eva Dyllong (Universität Duisburg-Essen, Germany) GA/CT3124/001

Among other approaches, such as implicit surfaces, constructive solid geometry or boundary representations, octrees feature a powerfull technique for the geometric modeling of rigid objects. A multi body system can be modeled with a composition of octrees for an efficient collision detection or collision prevention applications.

In this paper, we provide an algorithm for a reliable distance calculation of octree encoded objects. The algorithm is based on previous algorithms of Dyllong and Luther and has running times that are considerably shorter in different case scenarios, particularly in the worst case scenario.

GA/CTS4891/01: Non-smooth dynamics.

Organiser: Klaus Zimmermann (TU Ilmenau, Germany)
Co-organiser: Martin Arnold (Universität Halle-Wittenberg, Germany)
Co-organiser: Hartmut Bremer (Universität Linz, Austria)

Theory and experiments for distant effects in impacts. **Christoph Glocker** (ETH Zürich, Switzerland), Ueli Aeberhard (ETH Zürich, Switzerland), Matthias Payr (ETH Zürich, Switzerland) GA/CT1608/001

The paper addresses the question of non-localizable constitutive laws in Lagrangian impact dynamics. By setting up the kinematic, kinetic and energetic consistency conditions for frictionless multi-impact configurations, a set of admissible post-impact velocities is identified which generalizes the concept of perfect unilateral constraints to impulsive motion. Based on this set, impacts are classified with respect to their topology, intensity and dissipation behavior. Of particular importance for this classification is Moreau's half-line of local impact effects, which meets on its end the point of maximal dissipation. To address impacts with distant effects which are events apart from this line, Fremond's approach of setting up a matrix of restitution coefficients is carried out by a proper parameterization of the admissible post-impact velocity set. After having treated the scleronomic case, the theory is extended to configurations with uniform and non-uniform kinematic excitation, followed by a discussion of problems arising in systems with kinetic excitation. Measurements have been performed on Newton's cradle with three up to five balls, but also on longitudinal bars to experimentally validate the concept of prefect unilateral impulsive constraints, in particular in view of distant effects. For the evaluation of the experimental data, a mass-orthogonal decomposition of the impact in the spirit of constrained motion in classical mechanics has been performed. It decomposes the impact into impact-invariant directions with generalized momentum conservation and into directions which may be affected by the impact event.

On the Euler-Maupertuis principle of least action. **Remco Leine** (ETH Zürich, Switzerland), Ueli Aeberhard (ETH Zürich, Switzerland) GA/CT2109/001

Usually, Hamilton's Principle is used to derive the Lagrange's equations of motion (or vice versa), which yield second-order differential equations in time t and allow us to obtain the temporal solution curve $\mathbf{r}(t) = \begin{bmatrix} x(t) & y(t) \end{bmatrix}^{\mathrm{T}}$ for a mass m in a (2D) potential field. Starting from Hamilton's Principle, the current paper discusses how we can derive the Euler-Maupertuis Principle of Least Action (abbr. PLA)

$$\sqrt{2m}\int_{x_0}^{x_1}\sqrt{E-V(x,y)}\sqrt{1+y'(x)^2}dx = \text{stationary}, \qquad E = T+V = \text{const.}$$

which is sometimes called the Principle of Jacobi. This variational principle allows us to *directly* obtain the space curve $y(x)$ of the mass m in the potential field $V(x,y)$ without referring to the temporal dynamics. Alternatively, the PLA can be used for the inverse problem: find a robot/machine which realises a certain spatial curve $y(x)$ of its end-effector. The PLA dates back to Euler and Maupertuis and is the ancestor of Hamilton's Principle. Although the PLA is well known in theoretical physics, it seems to be almost forgotten in analytical dynamics. The aim of the paper is threefold. First, a historical overview of the PLA is given and its relation with Fermat's Principle is explained. Secondly, the use of the PLA in analytical dynamics is shown and the principle is applied to the looping curve of constant normal reaction. Thirdly, the PLA is put in the context of non-smooth dynamics, giving the principle a novel application field.

A parameterisation of impact laws in perfect multi-contact collisions. **Ueli Aeberhard** (ETH Zürich, Switzerland), Christoph Glocker (ETH Zürich, Switzerland) GA/CT2202/001

Impacts in rigid multibody systems cause instantaneous jumps in the generalised velocities. Naturally, the velocity after impact depends on the chosen impact law. An impact law should fulfil kinematic, kinetic as well as energy restrictions. In this paper, we study the domain of possible post-impact velocities for *arbitrary* impact laws. For single-contact collisions, this domain is at most one-dimensional but the domain becomes higher dimensional in the multi-contact case. The domain of possible post-impact velocities is a compact convex subset of the tangent space to the configuration manifold. Using a complete canonical parameterisation, the post-impact velocity of all impact laws can be addressed. For instance, the impact law corresponding to maximal dissipation as well as Newtons (extended) impact law are examples of incomplete canonical parameterisations. These impact laws are not complete as non-local impact effects are not addressed. Here, we try to find a complete canonical parameterisation which covers non-local impact effects. Moreover, the relationship between symmetries and conservation laws in this context will be elucidated.

Hammering in gear wheels. **Peter Eberhard** (Universität Stuttgart, Germany), Pascal Ziegler (Universität Stuttgart, Germany) GA/CT3977/001

The dynamic behavior of gear trains in Diesel engines is very often accompanied by a rattling motion of teeth within the backlash, called gear hammering. It originates in a transmitted mean torque that is small compared to dynamic loads introduced by gas forces, for example. Therefore the flanks are likely to lift off and reestablish impact-like contacts on both sides of the flanks causing a hammering noise. Clearly, the precise knowledge of these contact forces is very important for gear design. Typically, in industrial practise rigid body models are used to simulate these contacts, even though they have been developed for the investigation of sliding contact instead of impacts. Furthermore, since in gear trains the gears are often thin to reduce inertia, the compliance of the gear body influences the contact behavior significantly. Contact investigations of gears using transient finite element models reveal that in fact the gear body compliance may strongly influence the contact behavior and that dynamic gear body effects must be considered for precise simulations of contact forces. Since rigid body body models can not account for such effects and finite element models can only be used for some few impacts due to the huge numerical effort, a modal approach is proposed, where the gear wheel dynamics is described in a modally reduced formulation using a moving frame of reference. In combination with collision detection and a local force law, this approach allows very precise investigations of contact problems. Moreover, since all necessary data is determined in preanalyses, the integration is numerically extremely efficient. To validate this approach, experiments of test bodies impacting teeth of real gears have been carried out and compared to simulation results and a very good agreement is observed. Therefore, this approach offers a validated and precise contact model that is numerically efficient enough to be incorporated into overall engine models.

Impacts on 1D structures. **Roland Zander** (TU München, Germany), Heinz Ulbrich (TU München, Germany) GA/CT2865/001

Instancing the Woodpecker toy, which is a classic example for non-smooth mechanical behaviour, a description for the two and three-dimensional behaviour of slender elastic structures in presence of colliding bodies is developed. A special focus is laid on the discretisation of the elasticity, where different approaches can yield different advantages: the classical approach within flexible multibody systems (MBS) are global shape functions describing the deformation of the entire structure with respect to the discrete degrees of freedom. This gives a well defined limitation of the frequencies described within the model but is – in contrast to FE-approaches – insufficient to describe locally bounded effects like impacts on the structure. Here the FEM gives a locally bounded description.

The effect of modelling the flexibility of structures with impacts then is studied on the model of the Woodpecker toy: the rod representing the trunk is modelled as rigid followed by elastic models allowing for two and three-dimensional dynamics. In case of the elastic model, the Woodpeckers oscillation changes due to the interference with the structures oscillation. This structural vibration is induced and highly influenced by the Woodpeckers movements which continuously change the boundary conditions one the structure. This can be interpreted as changing mass distribution on the structure. When using a rigid model for the rod this effect is not included in the model.

This academic example of the woodpecker toy is presented since it holds all effects of interest for non-smooth dynamics of MBS: smooth mechanical parts, impacts and structural elasticities. At the same time it is simple enough to allow for judging the results obtained based on everyday experience. The methods and models described here can be used for the simulation of drive-trains, continuous variable transmissions (CVTs) and other machine parts.

02, Minisymposia

GA/MP396/002: Mechanical properties of biomembranes.

Organiser: Matthias Röger (MPI Leipzig, Germany)
Co-organiser: Rumiana Dimova (Max Planck Institute of Colloids and Interfaces, Germany)

Cell membranes constitute a basic structure of biological systems and have been a focus of scientific research over the years. Their complex architecture and the variety of processes involved explain the vitality of the subject as well as the difficulties that emerge in their analysis. A combined effort from different disciplines is often necessary to achieve a better understanding. In this minisymposium we will focus on a very few specific aspects with contributions both from biophysics and mathematical analysis.

Lipids and other amphiphilic molecules self-assemble into thin bilayers, which are the building blocks for many components of living systems. These five nanometer thick bilayers build the walls of cells and other cellular organelles. Under normal circumstances, lipid bilayers and biomembranes are not rigid but rather flexible and, thus, undergo thermally excited shape fluctuations such as protrusion modes or bending undulations. The latter give rise to a variety of shape transformation in vesicles.

Membranes within biological systems interact with many macromolecules. For example, on the inner surface, the plasma membrane is attached to networks of relatively stiff filaments which are part of the cytoskeleton inside the cell. A model system for these complex interactions is provided by systems containing lipid bilayers and polymers. Thus, the interaction of membranes with various molecules and particles has been addressed in theoretical analysis and simulations.

Even the fundamental processes in simple model systems pose an interesting challenge for a mathematical analysis. The self-assembling of lipid molecules into thin surface-like structures sharing both a solid-like and a fluid-like character is one example. Phase separation processes coupling the shape of a membrane to diffusion or coarsening on their surface is another one.

Phase separation in biomembranes: a diffuse interface approach. **Axel Voigt** (FZ caesar, Germany) GA/MT4021/002

Biological membranes form the interface between cells and its environment. They are a mixture of many different types of lipidic and protein components, and their relative amounts and composition differ between functionally distinct domains and changes dynamically during such processes as movement, division and vesicle trafficking. The local curvature has been recognized as a key parameter that might be related to precise biological properties. Various mechanism have been identified, which can generate positive or negative curvature, among these are: a) changes in lipid concentration, b) cytosceletal assemly and c) scaffolding by proteins. Even if all desired molecular informations were available, the computer time required to describe these interactions would be totally prohibitive.

A mathematical description which links microscopic morphology and biological function, thus should have the curvature as a key ingredient. Most studies on continuum models in this direction have been concerned with equilibrium shapes. Dynamic models are much more involved as they require a complex coupling between surface evolution, lipid composition and protein diffusion, which leads to highly nonlinear partial differential equations on evolving surfaces. The solution of such problems requires special care on the discretization and its theory is much less developed than for problems on Cartesian grids.

We develop for a thermodynamically consistent model for multicomponent lipid membranes a diffuse interface approximation which circumvents these technical difficulties and in addition allows to deal with topological changes.

Visualizing the dynamics of soft matter: membranes, nano-particles and vesicle fusion. **Julian Shillcock** (Max Planck Institute of Colloids and Interfaces, Germany) IC/MT4109/002

Biological membranes have properties and behaviour that emerge from the propagation across many scales of the molecular characteristics of their constituents. Artificial smart materials, such as drug delivery vehicles and biosensors, often rely on modifying naturally-occurring soft matter, such as polymers and lipid vesicles, so that they possess useful behaviour. Mesoscopic simulations allow in silico experiments to be easily and cheaply performed on complex, soft materials requiring as input only the molecular structure of the constituents at a coarse-grained level. Additionally, mesoscopic simulations provide the only currently feasible window on the length and time scales relevant to important biophysical processes such as vesicle fusion. We present recent work using Dissipative Particle Dynamics (DPD) simulations to explore the structure and behaviour of amphiphilic membranes, the fusion of vesicles, and the interactions between rigid nanoparticles and soft surfaces.

Membrane deformation under polymer pressure. **Carlos Marques** (CNRS-Institut Charles Sadron, France) GA/MT4077/002

Polymers and membranes are the one and the two-dimensional archetypes of the soft objects that compose the colloidal world. Ubiquitous in the living realm and in many industry formulations, these fluctuating ropes and sheets display a fascinating behaviour that has inspired many developments at the forefront of present nanotechnology trends. Soft Condensed Matter objects such as those made from polymers and membranes are easily deformed by viscous, electric, magnetic or gravitational forces. They also exhibit thermal fluctuations. This susceptibility to weak forces provides many pathways for structuring and patterning a range of nanostructures from soft materials Here I will present recent theoretical and experimental progress in the understanding of membrane behaviour under polymer stress.

I will first show theoretically what forces are expected when a polymer and a membrane are brought into interaction range, and compute the deformation of the membrane under polymer pressure. I will then present recent experimental progress from systems of phospholipid giant vesicles spread on a DNA carpet.

A mesoscopic model for cell membranes. **Matthias Röger** (MPI Leipzig, Germany) GA/MT4050/002

We derive a mesoscopic model for membranes formed by amphiphilic molecules. Such molecules consists of a polar *head* and a non-polar *tail* and self-assemble into surface-like structures. Starting from a microscopic description we obtain an energy defined on densities of head- and tail-groups. A mathematical analysis shows that this *mesocsale-energy* reflects the basic mechanical properties of cell membranes and is connected to a classical bending energies.

This is work done in collaboration with Mark A. Peletier (University of Technology, Eindhoven).

02, Short Communications

GA/CTS4444/02: **Soft tissues.**

Organiser: Wolfgang Ehlers (Universität Stuttgart, Germany)
Co-organiser: Philippe Zysset (TU Wien, Austria)
Co-organiser: Udo Nackenhorst (Leibniz Universität Hannover, Germany)

Large-scale simulation of arterial walls: mechanical modeling. **Dominik Brands** (Universität Duisburg-Essen, Germany), Jörg Schröder (Universität Duisburg-Essen, Germany), Daniel Balzani (Universität Duisburg-Essen, Germany), Axel Klawonn (Universität Duisburg-Essen, Germany), Oliver Rheinbach (Universität Duisburg-Essen, Germany) GA/CT1840/002

Biological soft tissues appearing in arterial walls are characterized by a nearly incompressible, anisotropic hyperelastic material behavior in the physiological range of deformations. For the representation of such materials we apply a polyconvex strain energy function, cf. [1], in order to ensure the existence of minimizers [2] and in order to satisfy the Legendre-Hadamard condition automatically. To account for the anisotropy the concept of structural tensors and representation theorems for anisotropic tensor functions are used and the energy is formulated in terms of the principle and mixed invariants of the deformation and structural tensor.

When arteries are overstretched, discontinuous damage is observed. For the modeling of this effect we apply a damage model specified in [3], which basically assumes that the damage occurs mainly in fiber direction. For the numerical simulation we consider an atherosclerotic artery and apply a high internal pressure which is comparable to the pressure applied during a balloon-angioplasty.

The 3D-discretization results in a large system of equations, therefore, a parallel algorithm using FETI-DP is applied to solve the equilibrium problem. The details of the domain decomposition method applied to this problem are discussed in a talk by O. Rheinbach.

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Discussion on appropriate material parameters for a porous media model of the IVD. **Nils Karajan** (Universität Stuttgart, Germany), Wolfgang Ehlers (Universität Stuttgart, Germany), Bernd Markert (Universität Stuttgart, Germany) GA/CT3992/002

In general, the intervertebral disc is known to be a representative of charged hydrated soft tissues, thereby exhibiting several coupled dissipative effects resulting from distinct swelling properties, interstitial fluid flow as well as an intrinsic viscoelastic extracellular matrix. Furthermore, its unique structure is dominated by embedded collagen fibers yielding a very efficient load bearing mechanism. In the past, it has been proved that a model based on the Theory of Porous Media (TPM) comprises a very efficient treatment of all the necessary characteristics which can be merged in a modular manner. However, regarding experiments on tissue specimens, it is often not possible to separate the involved effects as it is the case for the theoretical model. Hence, one of the main problems is the identification of the theoretically introduced material parameters. Moreover, the model includes certain structural properties, such as the fiber orientation or the fixed charges density, which are inhomogeneously distributed over the tissue. They can often be easily observed, and integrated into the model, but the relevance of these inhomogeneities to certain deformation modes of the IVD remains unknown. The goal of this contribution is to quantify the above mentioned problems and to discuss the possibilities for a reasonable parameter identification as well as a judgment of their influences.

Simulations of hydrated media with implicit Dirichlet boundary conditions. **Ayhan Acartürk** (Universität Stuttgart, Germany), Wolfgang Ehlers (Universität Stuttgart, Germany), Bernd Markert (Universität Stuttgart, Germany) GA/CT3978/002

Charged hydrated porous media, which are found in biomechanics as well as in geomechanics, have the capability to change their volume under varying chemical conditions of the environment. In this contribution these materials are modelled in the framework of the thermodynamically consistent Theory of Porous Media (TPM). The advantage of such a continuum mechanical model is that neither the porous micro structure nor the geometrical distribution of the constituents must be known.

The model underlying consists of four constituents, a charged solid and an aqueous solution composed of water and the ions of dissolved salt. The solid is modelled by a finite elasticity law accounting for the multiphasic micro structure, whereas the fluid is considered as a viscous *Newton*ian fluid. One finally ends up with four balance relations, the volume balance of the fluid, the concentration balance of the cations, the momentum balance and the balance of charges of the overall mixture.

The resulting set of partial differential equations is solved within the framework of the FEM. Therefore, the weak forms are derived and the resulting set of equations for the primary variables pore pressure p, cation concentration c and solid displacement $\mathbf{u}_S$, is implemented into the FE tool PANDAS. Finally, a three dimensional example is shown.

Material stability aspects for viscoelastic collagen fibers. **Bernd Markert** (Universität Stuttgart, Germany) GA/CT4009/002

The continuum mechanical modeling and predictive simulation of fibrous biological tissues, such as tendons, ligaments, skin etc., is of common interest in the field of computational biomechanics. In this regard, various strain-energies have been proposed to capture the inherent anisotropy caused by the aligned collagen fibers ranging from simple exponential functions to more sophisticated formulations based on the theory of invariants (see quotations in [1]) which are well established in macroscopic models of arterial walls and spinal discs.

The specific goal of this contribution is to describe the apparent relaxation and creep response of type I collagen fibers under tension which is believed to result from subfibrillar slippage mechanisms, whereas the elastic properties are brought into connection with the flexible regions in the collagen D-period [2]. Therefore, proceeding from a general polynomial-type strain-energy function formulated in the fiber stretch [1], the multiplicative geometric concept of finite solid viscoelasticity is applied in the framework of thermodynamics with internal state variables. In particular, the strain energy and thus, the stress are constitutively split into equilibrium and non-equilibrium parts governing the elastic and the rate-dependent fiber response. The evolution of the inelastic fiber deforma-

tion is thereby described by a thermodynamically consistent rate equation (viscoelastic flow rule) which remains valid even for large perturbations away from thermodynamic equilibrium. Moreover, the concise formulation still meets the requirements of a stress-free reference state and material stability, whereas the number of material parameters is kept to a minimum.

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A multiphase theory for the description of remodeling and growth in anisotropic living tissues. **Tim Ricken** (Universität Duisburg-Essen, Germany) GA/CT2337/002

The continuous capability of soft and hard living tissue to optimize their inner structure and material properties by growth, remodeling and morphogenesis is currently under study by groups of mechanic, biology, medicine and chemistry. Although a wide knowledge regarding the mechanisms being involved has been improved, it came out that these phenomena are extensively complex and of multi-scale dimension. A common approach is to assume that the tissue reacts to either stress, strain or even the rate of one of these effects. Models based on these assumptions may lead to good results, e.g. strain which induces bone remodeling or stress inducing remodeling and growth of soft tissue. Nevertheless, it is beyond dispute, that in addition to the stress or strain state, there are additional mechanisms which affect the remodeling and growth of biological tissues, e.g. growth factors or other dissolved solutes in the non-viscous fluid and the solid matrix. Due to the fact that tissue is composed of several components, in this contribution a multi-phase theory will be presented. The growth and remodeling mechanism is treated using a coupled description where several phases are involved. In order to formulate thermodynamic consistent restrictions, a closed system approach is being used. As a direct consequence, the validity of the mixture mass balance can be guaranteed without the introduction of a surface mass flux. Under consideration of the additional information captured by the coupled multiphase description, a new approach for the phenomena of growth and remodeling will be discussed. After presenting the developed framework for the calculation concept which is describing a growth in anisotropic biological tissues, some representative numerical examples are being examined.

Deformation of bilayer lipid membranes in bio-inspired materials and systems. **Raffaella De Vita** (Virginia Tech, USA) GA/CT4363/002

Bilayer lipid membranes (BLMs) have been successfully used in numerous medical, defense, and engineering applications such as drug delivery systems, sensors for detecting biological agents, and photovoltaic cells. Despite the fact that BLMs offer great promise for many applications, only few experimental investigations have been conducted to characterize their mechanics. Performing mechanical experiments is very challenging due to the poor stability and nanometer size thickness of BLMs. Therefore, the formulation of mathematical models becomes crucial not only in understanding the mechanical behavior of these lipid assemblies but also in guiding the design of suitable experiments.

A mathematical model will be presented to describe the deformation of planar BLMs that constitute many bio-inspired materials and systems. The BLM is assumed to be a Smectic A liquid crystal. Thus, the mean orientation of the amphiphilic molecules comprising the BLM is postulated to be perpendicular to the layers. Each layer is idealized as a two dimensional liquid. The small deflections of simply supported BLMs subjected to pressure loads that act perpendicularly to the layers are studied. The equilibrium equations and boundary conditions are derived from the bulk elastic energy proposed by de Gennes and Prost (1993) by using variational methods. The solution of the fourth-order differential equation for the resulting boundary value problem is found analytically by using cylindrical functions and their mathematical properties. *Work done in collaboration with Iain W. Stewart.*

GA/CTS4509/02: Cardiovascular.

Organiser: Alfred Kluwick (TU Wien, Austria)
Co-organiser: Philippe Zysset (TU Wien, Austria)
Co-organiser: Udo Nackenhorst (Leibniz Universität Hannover, Germany)

Modeling the cerebral blood flow using a multiscale finite-volume approach. **Johannes Reichold** (ETH Zürich, Switzerland), Alfred Buck (Universitätspital Zürich, Switzerland), Bruno Weber (Inst for Pharmacology and Toxicology, Universit, Switzerland), Patrick Jenny (ETH Zürich, Switzerland) GA/CT1956/002

Cerebral blood flow (CBF) can be defined as the rate of delivery of arterial (nutritive) blood to the capillary beds of a particular mass of brain tissue. CBF assumes a fundamental role in homeostasis and neural activity as it regulates the supply of glucose and oxygen.

A multiscale finite volume method is employed to model CBF in a realistic vascular network. High-resolution 3D data of the cerebral angioarchitecture in animal models acquired by Weber et al. [1] are utilized. The imaged blood vessels are divided into groups of large, medium and small lumen. While large and medium vessels are fully resolved, the capillary bed is modeled as an isotropic grid. Pressure is assumed to be constant in the large vessels while it may vary for smaller sizes. Other vessel properties such as diameter and curvature are represented by a corresponding transmissibility value.

Vasodilation during neural activity or partial occlusion in cerebrovascular impairment are examples of localized changes in vessel attributes. It is investigated how these local alterations affect the global CBF. Among others, insights gained from the simulations are valuable for the correct interpretation of data acquired by magnetic resonance imaging modalities. In addition, the validity of the description of blood as a Newtonian fluid is tested for various conditions.

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Dynamics of blood flow in the Willis circle using a quemada mode. **Adrian Postelnicu** (Universitatea Transilvania din Brasov, Romania) GA/CT3376/002

The Willis polygon (or Willis circle) is an arterial system, located at the base of the brain, which represents a security biological device. The paper presents new results on the dynamics of blood flow in the Willis circle, by taking into account the non-Newtonian nature of the blood through a Quemada model [3]. In previous papers [1-2] we performed a steady analysis of the blood flow in the Willis polygon, by considering the blood as a Newtonian fluid. In hemodynamics this is the first step, while taking into account the non-Newtonian behaviour of the fluid is called a second order approach. This is in fact the aim of our paper, to compare the results (blood flow rates and pressures) obtained in a non-Newtonian approach with those furnished by a Newtonian modeling of the blood.

This model is embedded in a standard analysis of a complex network of pipes, which is in fact the Willis circle from the hemodynamics point of view, by using a Quemada non-Newtonian model, as presented in [4]. Flow-rates in the arteries and pressures in their junctions are obtained and are compared with those corresponding to the Newtonian case. Then, in a second step, we extend our analysis to the unsteady flow in the Willis circle.

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Novel method of pulse wave diagnostics based on compression of a superficial artery. **Natalya Kizilova** (Kharkov Polytechnic University, Ukraine) GA/CT389/002

Wave propagation in the arteries is widely investigated in application to medical diagnostics. Determination of the diagnostically important parameters and their biomechanical interpretation are connected with mathematical approach to data analysis and solution of the corresponding coupled problem for the blood flow and vessel wall movement. Some novel aspects of the wave propagation in the arteries are connected with wave separation into their forward and backward running components, wave-intensity analysis, analysis of the resonant harmonics and the pressure-flow P(U) curves. Pulse wave propagation and reflection in a series connection of a viscoelastic tube and two complex resistances is considered as a model of the intraorgen arterial vasculature. Expression for the input admittance of the system taking into account wave reflection at the end of the tube is obtained. The dependence of the input admittance on the geometrical and mechanical parameters of the system is investigated. The equation for calculation the harmonics at which the input admittance reaches its extreme is obtained. The harmonics is considered as resonant, when any alteration in terminal admittance causes significant variation in the amplitude. The influence of variations of the model parameters within the physiological range on the amplitude and the phase spectra of the input admittance is investigated. The outer compression of the artery during the pulse palpation procedure is modeled as non-uniform pressure distribution at the outer surface of the tube. The parameters of the pressure wave (the modulus and phases of different harmonics) at the inlet of the system contain all possible information on the state (normal or pathological) of the inner organs. It is shown that at a proper slight or deep compression some harmonics may be amplified while the others are attenuated. Based on the theory of the so-called resonant harmonics of different inner organs the novel method of pulse wave palpation is proposed. The results are compared to other methods like separation of the pressure wave into its forward and backward components, estimation of the parameters of the reflected wave and wave-intensity analysis.

The modelling and dynamic analysis of flow through the aortic valve during the cardiac cycle. **Krzysztof Patralski** (Wroclaw University of Technology, Poland), Piotr Konderla (Wroclaw University of Technology, Poland) GA/CT4208/002

In mechanical terms the human heart is a kind of pump. During pulsation, the heart pumps blood around the body trough the circulatory system. The direction of blood flows and the mode of blood inflow into the ventricles are controlled by four valves which act as non-return valves. The object under study is an aortic valve, located in the aortic annulus. The main goal of this study is to consider the dynamic function of the model that consists of the aortic valve and the aortic artery wall model. Simulation is assumed to reflect the natural conditions of the flow through the valve. The earlier studies are presented[1,2].

The valve is composed of three spherical cusps connected to the common ring. Each leaflet is built of three layers. The aortic artery wall model is characterized by comosite structure. This objects are treated as the three symmetry plane objects. We assumed the hiperelastic Mooney–Rivlin material model. Fluid is assumed as incompressible Newtonian model. The dynamic density coefficient η = const. The load is variable in time.

The analysis problem is solved numerically by using FEM[3]. The computations were performed using the Ansys Multiphysics system. The fluid–structure interaction process is modelled using ALE method (Arbitrary Lagrange Euler).

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GA/CTS4445/02: Whole body, gait and spine.

Organiser: Udo Nackenhorst (Leibniz Universität Hannover, Germany)
Co-organiser: Philippe Zysset (TU Wien, Austria)

A sensitivity analysis of the Hill muscle model with respect to gait dynamics. **Daniel Strobach** (Universität Duisburg–Essen, Germany), Andres Kecskemethy (Universität Duisburg–Essen, Germany) GA/CT2232/002

This paper analyzes and quantifies the sensitivity of the Hill-type actuator model with respect to its characteristic parameters. It focuses on the influence of parameter variations in the context of forward dynamics simulations of muskuloskeletal motor tasks. The analysis is performed using a simplified subsystem of the human leg consisting of pelvis, thigh shank and foot, interconnected by planar joints at hip, knee and ankle. The system comprises one antagonistic muscle pair at the

knee for knee flexion and extension (*vastus intermedius* and *biceps femoris caput brevis*). The activation of muscle is modeled using a simplified parameterization based on smooth profile patches. To simulate the swing phase of gait, rheonomic constraints are imposed on pelvis (translation and rotation), hip (rotation) and ankle (rotation). The paper shows that the different parameters involved in the muscle model can have significant varying influence on the resulting behaviour, showing which parameters need to be determined accurately and which allow for a more rough estimation.

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A comparison of static optimization criteria for resolving the muscle-redundancy problem during human gait. **Ye Ou** (Universität Duisburg–Essen, Germany), Andres Kecskemethy (Universität Duisburg–Essen, Germany) GA/CT2273/002

In human movement, several muscles activate a single degree of freedom, leading to the problem of force redundancy. To resolve this, static optimization offers a computational advantage, while neglecting dynamic effects. However, such static optimization techniques often render suitable results, and are thus frequently found in biomechanics literature. In this paper, we investigate different approaches of static optimization for predicting the muscle forces. A four-segment linked leg musculoskeletal model with motion in the sagittal plane is considered. The joint moments generated by muscles are computed from inverse dynamics. The muscle force is estimated by different optimization criteria, each satisfying the moment constraints at all joints and the minimum and maximum muscle force constraints. Several criteria described in literature are studied using linear or nonlinear optimization. The results obtained from these calculations are compared with each other.

Reduced kinematic model of the human spine for biomechanic application. **Christian Simonidis** (GAMM, Germany), Wolfgang Seemann (Universität Karlsruhe, Germany), Manuel Scharmacher (Karlsruhe, Germany) GA/CT2418/002

Based on functional anatomy a detailed kinematic model of the human spine is developed. The human spine is an agile and adaptive mechanical system consisting of several biological components such as bones, ligaments and muscles. Thus it can be seen as a highly kinematic and dynamic coupled multibody structure, where the bones can be considered as rigid body elements. Intervertebral discs and facet joints form a defined relative motion range between two adjacent bodies. Ligaments as well as muscles couple the whole structure. The present kinematic coupled model has three degrees of freedom and represents the motion range of the biological system. Further, we define a substitutional joint for relative kinematics between vertebra prominens and pelvis allowing a motion range close to the motion range of a human torso. Results are verify by mapping motion capture data from motion study on the models.

Anatomically-based mechanical models of the human pelvic floor. **Leo Cheng** (University of Auckland, New Zealand), Kim Noakes (University of Auckland, New Zealand), Andrew Pullan (University of Auckland, New Zealand), Ian Bissett (University of Auckland, New Zealand) GA/CT4391/002

There are gaps in our understanding of the role of different muscles in the pelvic floor region and their relative contributions to maintaining continence and the normal defecation process. To address this deficiency, we have created anatomically realistic finite element (FE) models of the structures within the pelvic floor region.

The FE models were constructed from images of male and female cadavers from the Visible Human Project and MRI data from a normal live female subject. For each data set, up to 14 individual structures of interest were manually segmented from the axial images. Segmented points were then reviewed again against saggital and coronal images and also reviewed by an anatomist and a pelvic floor surgeon. FE representations of each of the structures were created using a non-linear fitting procedure that minimised the orthogonal distance between segmented points and the FE mesh to produce an RMS error of less than 1.1 mm.

A 'bear down' or abdominal squeeze was simulated on the levator ani (LA) muscle of the live subject by solving the governing finite elasticity equations. The LA muscle was represented by a 160 node FE mesh with tricubic Hermite interpolation and an isotropic two parameter Mooney-Rivlin material law. Boundary conditions were applied to represent the in vivo conditions. Nodes at the posterior of the LA muscle that corresponded to points attached to the coccyx bone had all displacements fixed and nodes that corresponded to the portions attached to the fasciae of the obturator internus muscles were constrained to move only the superior-inferior direction. A pressure of 4 kPa (corresponding to an average supine intra-abdominal pressure during valsalva) was applied to the superior surface of the LA muscle and the resulting deformation computed. The simulated data was correlated against a dynamic, saggital MR image obtained from the same subject during the valsalva manoeuvre.

Study of human body stability under the vertical vibration action into an autovehicle using Laplace transforms. **Mariana Arghir** (Universitatea Tehnicã Cluj-Napoca, Romania), Simona Rodean (Universitatea Tehnicã Cluj-Napoca, Romania) GA/CT1155/002

We present a study for imagining of generalized mechanical model for the human body / seat assembly. The model will by used for the dynamics analyze of the human body constituent parts, under the vertical vibrations influence, transmitted by the vehicle seat during its displacement. Measures of the dynamic responses of the body are represented by the transfer functions. The human body can be considered as a mechanical system and it may be roughly approximated by a linear lumped parameter at low frequencies (less than $100\,\mathrm{Hz}$) and low vibration levels. The resonance phenomenon appears due of the interaction of the concentrated masses with the pure elastically structure. This model is needed to investigate the human response to vibrations. The mechanical model of human body is defined in terms of discrete masses, dampers and springs.

Under the vibration action, the human body multiplies or diminishes the vibrations magnitude in accordance with mechanical vibration laws, as a mechanical system with mass, elasticity and damping characteristics. This is a mechanical model of the human sits upright on the seat cushion on the seat and consists of four parts: pelvis, upper torso, viscera and head. Therefore, the model has 5 DOFs in translation, where 4 DOFs represent the human body constituent parts and 1 DOF is for the seat cushion. Applying Laplace Transforms, the motion

differential equations system writing in time domain becomes an equivalent algebraic system in frequency domain, which is frequency response function of system and is expressed by the $H(s)$ transfer matrix and them transfer functions. Stability of the human body is established using the found poles. The human body motion laws with four independent coordinates are given in a graphical representation.

GA/CTS4446/02: Muscle and bone.

Organiser: Philippe Zysset (TU Wien, Austria)
Co-organiser: Udo Nackenhorst (Leibniz Universität Hannover, Germany)

Bridging scales: an attempt to incorporate cellular responses within a 3D FEM model of active muscle contraction. **Oliver Röhrle** (University of Auckland, New Zealand), John Davidson (University of Auckland, New Zealand), Juliana Kim (University of Auckland, New Zealand), Andrew Pullan (University of Auckland, New Zealand) GA/CT1373/002

Mathematical models representing skeletal muscles as 3D objects are rare. Most of them describe the contractile mechanics of skeletal muscles using the Finite Element method (FEM) to discretise the governing equations of finite elasticity and incorporating transversely isotropic constitutive laws, which mimic basic physiological properties of passive and active muscle mechanics.

Such models, however, are not capable of investigating the mechanical response of a muscle with respect to recruitment patterns, spatially varying contractions, or fatigue. To do so, it is essential to incorporate information from the cellular level. The challenge is thus to bridge and link information obtained from different scales specifically from the cellular level to the biomechanical FEM muscle model.

A mathematical model of the cellular responses of skeletal muscles has been integrated within a 3D biomechanical FEM model. For each muscle fibre, the skeletal cell model is able to reproduce a number of cellular properties including the action potentials of the sarcolemma and T-tubule, Ca^{2+} concentrations, and fatigue responses. The FEM model is based on a cubic Hermite Finite Element discretisation of the governing equations of finite elasticity theory and a transversely isotropic constitutive law.

To incorporate the cellular information into the FEM model, homogenised values of key physiological parameters, e.g. the calcium concentrations, are computed at Gauss points. These values are then used to modify the stress tensor in such a way that it resembles its contractile response. The methodology is applied to simulate the mechanical response of the semitendinosus after a nerve stimulus initiates muscle contraction.

The advantages of such an improved 3D FEM model are far reaching. These models can be used, for example, to investigate and study local muscle contraction, muscle recruitment patterns, force generation, or fatigue response of skeletal muscles.

Estimation of material properties of cancellous bone using multiscale FEM. **Sandra Ilic** (Ruhr-Universität Bochum, Germany), Klaus Hackl (Ruhr-Universität Bochum, Germany), Robert Gilbert (University of Delaware, USA) GA/CT2338/002

Cancellous bone is a spongy type of bone with voids filled by blood marrow. Without much loss of generality it can be modelled as a material with periodic microstructure where overall parameters can be calculated using some homogenization method. Here the multiscale finite element method is applied and the assumed representative volume element (RVE) is a cube with solid frame and fluid core. From the point of view of the finite element method the RVE is a combination of solid and shell elements with two types of boundary conditions. On the fluid-solid interface continuity of displacements orthogonal to this surface is required and as a consequence of the Hill-Mandel macrohomogeneity condition on the external boundary of the RVE periodic boundary conditions must be satisfied. We would like to consider acoustic excitation so that a complex stiffness matrix and complex displacements appear in the solution of the problem. Calculation of overall properties is repeated for different geometries of the solid frame.

Bearing of geometric and material properties to bone strength in bending. **Werner Winter** (Universität Erlangen–Nürnberg, Germany) GA/CT1841/002

Osteoporosis is characterized by decreasing of bone mass and bone strength with advanced age. For characterization of material properties of bone the volumetric bone mineral density (vBMD) is one of the most important contributing factors to bone strength. Often bending tests of whole bone are used to get information about the state of osteoporosis. From an uniaxial test of a bone specimen it is assumed that an elastic region exists up to initial yield stress and a following hardening region. In bending tests beside material properties geometric properties like shape and cortical thickness appropriate the non-linear load-deformation curves.

In a first step, different types of cellular structures are considered to characterize vBMD and its influence to elastic and plastic material properties. By scaling of the vBMD with the density of dense bone a relative volumetric bone mineral density can be regarded. Afterwards, the classical theory of plastic bending is used to describe the non-linear moment-curvature relation of a whole bone. For bending of bone with sandwich structure an effective moment of inertia can be defined. The shape factor as a pure geometrical value is considered to define bone strength due to bending in the non-linear range. This factor is discussed for a bone with circular cross section and different thickness of cortical bone. The deduced relations and the decrease of material properties are used to demonstrate the influence of osteoporosis to bone bending strength.

It can be shown that the elastic and plastic material properties of cellular bone are related to a relative volumetric bone mineral density. Starting from an elastic-plastic bone behavior with an constant yield stress the non-linear moment-curvature relation in bending is related to yielding of the fibres in the cross section. The ultimate moment is characterized by a shape factor depending on the geometry of a cross section.

About the necessity of extended remodeling theories in bone adaptation. **Tobias Ebinger** (Universität des Saarlandes, Germany), Stefan Diebels (Universität des Saarlandes, Germany), Holger Steeb (Universität des Saarlandes, Germany), Thorsten Tjardes (University Witten/Herdecke, Germany) GA/CT1706/002

At the moment an optimization process in the surgery of femoral neck fractures can be observed. While in former years mainly the complete head of the femur was replaced by an implant, now there is the trend to save the head if possible and to fixate it at the femur by screws. Thereby, numerical simulations provide the possibility of optimizing the position of the screws or of predicting failure under certain loading conditions.

Due to the complex microstructure of spongy bone (trabecular microstructure) deformation modes of higher order appear

leading to size effects. These higher order (e. g. bending-like) modes can not be reflected by standard continuum theories. Thus, continuum models considering higher order effects may be used to include such effects. However, that raises the question, if the extra effort is really needed, because the higher order deformation modes may avail failure, or – if unnecessary – it is blowing up the numerical cost only.

On the basis of a three dimensional anisotropic model for bone remodeling the need of extended biomechanical continuum models predicting failure is discussed.

Computation of statistically-equivalent load sets for bone-remodelling simulation. **André Lutz** (Universität Hannover, Germany) GA/CT2150/002

Theories and related computational techniques for the prediction of bone mass loss, for example caused by endoprosthetic treatment, are under discussion since more than 20 years. Today numerical aspects and constitutive modelling of stress adaptive bone remodelling seems to be solved sufficiently, but an open question arises from the description of the loading conditions in the framework of quasi-static approaches. Due to the complexity of the subject there is only a small data base available on measured and computed joint and muscle forces for typical movement situations. To close this gap an inverse simulation approach on the identification of statical equivalent load sets, related to measured bone mass density distributions, will be presented in this contribution. Based on a first order approach of bone remodelling, these load sets are computed by an hierarchical genetic-gradient algorithm and lead to the original bone mass distribution obtained by high resolution imaging techniques. Under consideration of these biomechanically equilibrated finite element models, computational results on the bone remodelling prediction due to treatment of artificial hip-joint replacement will be presented.

03, Short Communications

GA/CTS4771/03: Numerical methods (FEM 2).

Organiser: Klaus Hackl (Ruhr-Universität Bochum, Germany)
Co-organiser: Wolfgang Müller (TU Berlin, Germany)
Co-organiser: Dietmar Klingbeil (BAM Berlin, Germany)

A fully variational strong discontinuity approach at finite strains. **Radan Radulovic** (Ruhr-Universität Bochum, Germany), Jörn Mosler (Ruhr-Universität Bochum, Germany) GA/CT2212/003

A novel, fully variational three-dimensional finite element formulation for the modeling of locally embedded strong discontinuities at finite strains is presented. The proposed numerical model is based on the Enhanced Assumed Strain concept with an additive decomposition of the displacement gradient into a conforming and an enhanced part. The discontinuous component of the displacement field which is associated with the failure in the modeled structure is isolated in the enhanced part of the deformation gradient. In contrast to previous works, a variational constitutive update is used. The internal variables are determined by minimizing a pseudo-elastic potential. The advantages of such a formulation are well known, e.g. the tangent stiffness matrix is symmetric, standard optimization algorithms can be applied and it represents a natural fundament for error estimation and mesh adaption.

Finite-element formulations of shear localization in granular materials. **Tuyet Trinh** (Ruhr-Universität Bochum, Germany), Klaus Hackl (Ruhr-Universität Bochum, Germany) GA/CT3662/003

Displacement and mixed finite element formulations of shear localization in granular materials are presented. The formulations are based on hypoplastic constitutive laws for soils and the mixed-enhanced treatment involving displacement, strain and stress rates as independently varied fields. Included in these formulations are the standard displacement method, the three-field mixed formulation, the method of incompatible modes, the enhanced assumed strain method and the mixed enhanced strain method. Several numerical examples demonstrating the capability and performance of the different finite element formulations are presented. The numerical results are compared with available experimental data of Hostun RF sand and numerical results of Karlsruhe sand on biaxial tests.

Crack propagation calculation using trial cracks. **Martin Bäker** (TU Braunschweig, Germany) GA/CT1906/003

We present a method to perform finite element calculations for crack propagation problems with arbitrary crack directions in two dimensions. The crack direction (angle of propagation) is determined by inserting small “trial cracks” at the crack tip. For each trial crack, the domain is remeshed to allow crack propagation between elements. The trial cracks are then opened and the energy release rate is measured. The optimum crack direction (i.e., the crack direction with maximum energy release) is determined by an optimisation procedure. Although the method is computationally expensive due to the need to perform several calculations for each crack increment, it has the advantage that the energy release rate can be calculated even in cases where other methods fail. After explaining the method, it is applied to several test examples comparing it to other methods.

Creep damage anisotropy of thin-walled element structures. **Vyacheslav Burlayenko** (National Technical University ’Kharkov Polytechnic, Ukraine) GA/CT838/003

The talk is devoted to damage-induced due to a creep anisotropy (transversally-isotropic) of metallic materials under thermo-mechanical loading. Both types of an initially isotropic and anisotropic material were considered. For the description of initial anisotropy and damage-induced anisotropy the second-order damage tensor has been used. Constitutive equations are based on irreversible thermodynamics, namely the Helmholtz free energy. Theoretical results were compared with experimental data; the results of comparison were satisfactory. The proposed model was generalized to describe damage anisotropy (transversally-isotropic) and lifetime prediction in thin-walled elements of structures, using the engineering models of plates and shallow shells. The method of numerical simulation of an anisotropic creep damage analysis on the basis of finite element scheme was elaborated. Various creep properties of damage-induced anisotropy plates depending on the orientation of anisotropy axes of a material concerning to a direction of loading and from a degree initial anisotropy have been established.

Non-isothermal creep-damage model of heat-resistant steel. **Gennadiy Lvov** (Kharkov Polytechnic University, Ukraine), Evgen Kostenko (Dr.-Ing. Siemens AG Steam Turbine Technology, Germany) GA/CT773/003

Constructional elements of gas and steam turbines function in conditions of the high temperatures and complex loadings for a long time. Creep-damage analysis and determination of rupture time are the important part of turbine design. Numerous results of transient thermal analysis for high and low pressure turbine casing, exhaust casing and diffusers specify non-uniform character of distribution of temperatures that demands of non-isothermal creep and damage analysis. The purpose of this paper is to develop improved theory for heat-resistant steel and computer methods for calculate high temperature creep and damage of turbine components. Constitutional equations for ratio creep deformations and the kinetic equation of damage accumulation with continuous functional dependence on temperature are offered. For uniaxial stress behavior under constant stress and temperature the theoretical creep curves have first, second and tertiary stages. The technique of parameters verification for uniform model is developed on the basis of experimental creep curves and long-time strength in a wide range of temperature changes. Identification of the parameters in the non-isothermal creep-damage model, for one type of heat-resistant steel used in the turbine industry, is carried out. For numerical calculations of complex components of turbines the software is created, enabling using the developed model in FEM - program complexes. Calculations of creep are carried out and time rupture is found for elements of steam and gas turbines with use of various ways of the account of temperature change.

GA/CTS4773/03: Miscellaneous aspects of fracture and damage, I.

Organiser: Klaus Herrmann (Universität Paderborn, Germany)
Co-organiser: Wolfgang Müller (TU Berlin, Germany)
Co-organiser: Dietmar Klingbeil (BAM Berlin, Germany)

Fatigue life investigation using non-destructive testing methods. **Zoran Stankovic** (Ruhr-Universität Bochum, Germany), Otto Bruhns (Ruhr-Universität Bochum, Germany) GA/CT2186/003

Experimental investigation of the fatigue life prediction of two different specimen forms made from steel 42CrMo4 is described. The fatigue load was defined as a cyclic loading with constant and non constant amplitudes in tension range and with different stress ratios. This loading range leads to a high cyclic fatigue behaviour of both specimens. During the test, the growth of the fatigue crack was monitored using two different non-destructive methods, namely acoustic emission and the electric resistance. Acoustic emission was used for detecting sound waves as a result of dissipation of elastic energy during micro cracks and cracks growth, as well as for the detection of the place of crack initiation. Electric resistance was used for the monitoring and quantitative investigation of the crack growth.

On the effect of Kirkendall voids on solder-joint reliability. **Kerstin Weinberg** (TU Berlin, Germany), Thomas Böhme (TU Berlin, Germany), Wolfgang Müller (TU Berlin, Germany) GA/CT2515/003

Microelectronic circuit boards consist of the Si-chip itself and its packaging, which includes wiring and solder joints between different metal layers. Failure of these joints is a well established cause of failure of the whole circuit board. In addition to the challenges posed by the replacement of lead in solder joints the miniaturisation of microelectronic components is changing the failure mode of interest from conventional thermal cycling induced fatigue to drop impact induced solder joint fracture. Experimental evidence shows that the formation and growth of so-called Kirkendall voids significantly contributes to the degradation of solder joint strength and drop reliability.

For a continuum mechanical approach to such processes the question is: How can the additional information about the micro-structural development be included in a constitutive model? One possibility is the use of a general mesoscopic concept, firstly introduced by Muschik and his co-workers (see [1] and cited works) to describe a certain microstructure with continuum mechanical methods. The basic idea is the extension of the space-time domain by a set of mesoscopic variables. Additionally, a mesoscopic distribution function is introduced; in this way a statistical element enters the classical continuum theory.

By means of this mesoscopic theory we model a general viscoplastic solid material with a certain porosity. In this way it is possible to link the mechanisms of chemo-mechanical induced growth of voids to parameters which describe the macroscopic material softening. Numerical simulations provide inside into the (not yet completely understood) mechanisms of failure by formation and growth of Kirkendall voids.

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Identification of material symmetry for anisotropic damage evolution due to a growing mixed-mode crack. **Kianoush Molla-Abbasi** (Ruhr-Universität Bochum, Germany), Henning Schütte (Ruhr-Universität Bochum, Germany) GA/CT2209/003

A numerical study of a growing mixed-mode internal elliptical/circular crack in a unit cell was undertaken with the help of a finite element simulation. The model enables us to measure the components of the elastic compliance/stiffness tensor of the unit cell related to the principle loading axes as the crack grows. With this the evolution of the type of material symmetries and the evolution of the anisotropic damage are resulting.

The matrix of the unit cell is considered to be linearly elastic, homogenous and isotropic and the crack is small compared to the unit cell, so that the non-interacting crack assumption for damage models is fulfilled and the overall behavior of the unit cell is linearly elastic. This enables us to use linear elastic fracture mechanics (LEFM) concepts for the propagation of the microcrack.

The propagation of the crack is governed by the principle of maximum driving force which is a direct consequence of the variational principle of a cracked body in equilibrium and considers the effect of all three stress intensity factors. Without any ad hoc assumption, the crack growth rate is calculated using its thermodynamic duality with the local maximum driving force.

As the crack propagates, remeshing algorithm deletes the mesh, extends the crack and meshes the unit cell according to the new crack configuration. For each propagation step the components of the compliance tensor are calculated with the help of 6 basic deformation modes at which the unit-cell is either under pure shear or under pure tension. It is observed that the symmetry of the unit cell at each step of crack propagation is approximately orthotropic.

The impact of different fracture criteria on the evolution of the damage and the crack tip parameters are compared and the advantages of the maximum driving force criterion are discussed.

Keywords: anisotropic damage, compliance tensor, crack propagation, material symmetry

The effect of crack faces contact interaction on the critical strain in composites under compressive loading. **Bartlomiej Winiarski** (University of Aberdeen, UK), Igor Guz (University of Aberdeen, UK) GA/CT1188/003

Nowadays many primary structures in aviation and aerospace [1] applications are made of layered composite materials [2]. Components made of composite laminates due to their internal structure and manufacturing methods often contain a number of inter- and intra-component defects which size, dispersion and mutual interaction alter significantly the critical compression strain level [3]. The current study investigates the effect of the cracks interaction and crack faces contact interaction on the critical strain in laminar transversally isotropic material (cross-ply) compressed in a static manner along interlaminar defects. The frictionless Hertzian contact is considered for the interacting crack faces.

The statement of the problem is based on the most accurate approach, the model of piecewise-homogenous medium [4] and the 3-D stability theory. The moment of stability loss in the microstructure of material is treated as the onset of the fracture process. The complex non-classical fracture mechanics problem is solved utilizing the finite elements analysis. The results are obtained for the typical dispositions of cracks. It was found that the crack faces contact interaction alter significantly the critical strain level of the composite.

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Simulation of skin-stiffener debonding in stiffened curved carbon/epoxy panels. **Claudio Balzani** (Universität Karlsruhe (TH), Germany), Werner Wagner (Universität Karlsruhe, Germany) GA/CT1725/003

In the last decades, fiber-reinforced materials have obtained huge attention for high performance lightweight structures. Especially in the aircraft industry carbon/epoxy laminates play an important role due to their low weight paired with high stiffness and strength. But still there is a need for reliable and robust simulation tools in the design phase which incorporate evolutionary damage growth. One damage scenario which reduces significantly the load-carrying capacity of fuselage structures is the separation of the skin from the stiffeners. The aim of this presentation is the numerical treatment of this damage scenario in multi-directional carbon/epoxy panels in the framework of the finite element method. For this purpose, the composite itself is modelled with layered quadrilateral shell elements of Reissner-Mindlin type. For the description of skin-stiffener debonding isoparametric cohesive interface elements are derived. A cohesive law based on publications of de-Andrés et al. [1999] and Ortiz & Pandolfi [1999] is edited in a way that only tensile normal tractions trigger damage. Furthermore, the cohesive free energy function is enhanced by an additional penalty term in order to avoid the inter-penetration of the crack faces. Some numerical examples with experimental evidence demonstrate the applicability and the performance of the proposed model.

GA/CTS4774/03: Miscellaneous aspects of fracture and damage, II.

Organiser: Klaus Herrmann (Universität Paderborn, Germany)
Co-organiser: Wolfgang Müller (TU Berlin, Germany)
Co-organiser: Dietmar Klingbeil (BAM Berlin, Germany)

Material dispersion in dynamic deformation process of solids under impact action. **Adam Glema** (Poznan University of Technology, Poland) GA/CT3632/010

The dispersion as the solid material property is discussed in the paper. The phenomenon is well known from the point of view of wave analysis and is one of the main criteria for wave classification. Nevertheless mechanics of solids is still the branch of research and construction of mechanical and civil engineering structures, where dispersion and wave analysis play the minor role in process of conception, design, verification and production. The definition, origination and dispersion analysis in solids are presented. In the paper we concentrate on the mechanical behavior of solids. Wave nature, rate dependent material respond is the result of dynamic impact loading. The mechanical problem of inelastic deformation of solids is considered. The evolution of deformation under impact loading is described by rate dependent, hardening and softening viscoplastic model of material. The dispersion phenomenon is studied to introduce the adequate material model for the advanced states of deformation processes. The evolution problem is formulated within the frame of theory of thermodynamics and viscoplasticity. Mathematical analysis for elastic, plastic and viscoplastic material evidence the non-dispersive or dispersive property. Occurrence of dispersion in the analysis problem has the consequences not only for constitutive relation. It influences the whole problem with advantages in formulation and solution. Numerical results of example problems present qualitatively different mechanical response for materials with different dispersion. The formation of finite strain localization zone is controlled by viscous material parameters. Wave character and dispersion are recognized as fundamental elements in formulation and solution in dynamic processes with strain localization and shear band propagation. Physical and numerical aspects of dispersion clarify the development of deformation, stress or energy distribution and verify solution procedure. The dispersive character of material in analysis of plastic strain localization is essential and non neglectable phenomenon within solid mechanics problems.

Modeling of tear propagation in soft hydrated biological tissue. **Hans-Uwe Rempler** (Universität Stuttgart, Germany), Wolfgang Ehlers (Universität Stuttgart, Germany) GA/CT4020/002

Similar to dense solid materials, soft tissues tear due to strain overloading. However, the damage behavior (i.e., the tear expansion and propagation), also depends on the hydration of the tissue and may be affected by the interstitial fluid flow.

In this contribution, soft biological tissues are modeled using the Theory of Porous Media (TPM) which allows the description of multi-component continua with internal interaction. Here, the tissue is described by a standard two-phase model consisting of a solid matrix and an interstitial fluid. For the numerical treatment of the tearing mechanism, an extension of the Finite Element Method (X-FEM) is applied. In order to account for the increased fluid percolation in the opening tear, a special treatment of the permeability characteristics is required.

Within this framework, the influence of the pore-fluid flow on the tear propagation is examined in canoncial numerical examples.

Numerical analysis of chip formation during machining for different values of failure strain. **Jaroslaw Chodor** (Koszalin University of Technology, Poland), Leon Kukielka (Koszalin University of Technology, Poland) GA/CT2895/003

Machining is a very complicated technological process. To better understand the process of chip formation and various phenomena that can occur, we need to know what happens during machining. Separating material from base is one of the most important factors to be analysed, where the maximum value of failure strain is overflow. This value presents the stiffness of material after exceeding a particular limit, beyond which cracking and dividing of the material is observed. In the literature, this value typically falls within the range $\varepsilon_i = 0.25$ to 3, for various kinds of materials. Obtaining this value theoretically, and explaining its influence on the process of chip formation under experimental conditions, is a very difficult problem. Hence we proposed using some numerical analysis. Knowledge of the different values of failure strain allows observion of the critical moment within the chip-forming process, and how this value affects the state of strain and stress in the surface layer. We present results of numerical calculations for maps of strain and stress in the surface layer of actual work-pieces.

In this work attention is concentrated on chip formation and separation from the object for different values of the failure strain. The phenomena on a typical incremental step are described using a step-by-step procedure, within an updated Lagrangian formulation. Then finite element methods (FEM) and dynamic explicit methods (DEM) were used to obtain a solution. An application was developed in the ANSYS system, which makes possible a complex time analysis of the physical phenomena: states of displacements, strains and stress. Numerical computations require a proper definition of the contact zone by Single Surface Auto 2D, without the necessity to introduce boundary conditions.

The effect of fillet radius of the tool blade on the stress and strain states in the process of cutting a sheet plate with circular cutters. **Jan Bohdal** (Koszalin University of Technology, Poland), Leon Kukielka (Koszalin University of Technology, Poland) GA/CT3100/003

The influence of fillet radius of the tool blade on deformations and stresses of sheet metal in the process of cutting with numerical tools is presented. The Cowper-Symonds model is used to describe the properties of cut sheet-plate. Numerical results were obtained by the finite element method (FEM) making use of the ANSYS LS-DYNA ver. 9.0 program. The problem was approached using the central - difference method, also referred to as the explicit-integration method. It includes a few special techniques for direct integration of dynamic equations of motion.

GA/CTS4770/03: Numerical methods (FEM 1).

Organiser: Dietmar Klingbeil (BAM Berlin, Germany)
Co-organiser: Wolfgang Müller (TU Berlin, Germany)

Quasi-static crack propagation with X-FEM and material force method. **Jürgen Glaser** (TU Kaiserslautern, Germany), Paul Steinmann (TU Kaiserslautern, Germany) GA/CT2173/003

The presented work is based on the combination of two concepts being major subjects of computational fracture mechanics in recent time: The Material Force Method (MFM) and the Extended Finite Element Method (X-FEM).

The X-FEM modifies the standard Finite Element approach in order to describe the discontinuous displacement field across a crack (and the asymptotic crack-tip field) by the introduction of additional degrees of freedom (DOFs) at nodes in the vicinity of the crack. The displacement jump is modelled by a step function connected to those additional DOFs. The most obvious advantage of the X-FEM is the representation of a crack independently of the mesh such that no remeshing is needed in the case of crack propagation.

Material or configurational forces emanate from a balance law in material space which is connected to the material energy momentum tensor also called Eshelby stress tensor. The derivation of material forces is dual to the derivation of physical forces in the spatial configuration. In the case of a cracked specimen the MFM leads to a singular material force at the crack tip which is associated to a variation of the material placement of the crack tip and thus is interpreted as a driving force for crack propagation. The amount of that singular material force is equal to the J-integral of classical fracture mechanics.

Applying the MFM to FEM leads to discrete nodal material forces. The application of the Material Force Method to 2D quasi-static crack propagation within the framework of the X-FEM will be illustrated by several examples with a focus on the nodal material forces at standard degrees of freedom as a criterion for crack propagation. Examples for the geometrically linear and non-linear case will be presented and the question of how to determine the correct direction of crack propagation will be discussed.

Material force based mesh optimization in geometrically nonlinear hyper-elastostatics. **Michael Scherer** (TU Kaiserslautern, Germany), Paul Steinmann (TU Kaiserslautern, Germany) GA/CT2106/003

The aim of this work is the development of an r-adaptive scheme based on the concept of material forces. In the framework of the finite element method, the material force acting on a node of the material mesh corresponds to the gradient of the discrete potential energy with respect to the position of the node. Therefore, material forces provide the basis for r-adaptive methods that improve the finite element solution by minimizing the discrete potential energy.

The energy based mesh optimization can be considered as a minimization problem with constraints, whereas the constraints are given by the restriction that element degeneration must not occur. Based on this interpretation we developed a stable algorithm in which the distortion of the mesh is prevented by using an additional energy playing the role of a barrier function. The algorithm produces a sequence of meshes with decreasing potential energy and norm of the material node forces.

Beside the theoretical aspects and the implementation, a number of numerical experiments with triangular and tetrahedral meshes are presented. We discuss the advantage of the proposed r-adaptivity in the case of a notched and cracked specimen.

A computational framework of 3D configurational-force-driven crack propagation. **Ercan Gürses** (Universität Stuttgart, Germany), Christian Miehe (Universität Stuttgart, Germany) GA/CT4007/003

The lecture outlines a variational formulation of quasistatic brittle fracture in elastic solids and proposes a finite-element-based computational framework for propagation of cracks in three-dimensional bodies. The starting point is a variational setting of fracture mechanics that recasts a monotonic quasistatic fracture process into a sequence of incremental energy minimization problems. This extremum formulation includes the classical Griffith theory of brittle fracture. The proposed algorithm employs 4-noded linear tetrahedral elements and introduces discretized crack patterns with material-force-driven incremental nodal and crack surface releases. These releases of crack facets constitute a sequence of positive definite subproblems with successively decreasing overall stiffness, providing an extremely robust algorithmic setting in the postcritical range. The formulation is also embedded into an accompanying r-adaptive crack-pattern adjustment procedure with material-force-based indicators in conjunction with crack front constraints. The adjustment procedure allows reorientations of finite elements at the crack-front providing a considerable improvement in the predictions of *curved crack surfaces* when compared with the experimental observations. The capabilities of the proposed algorithm will be demonstrated by means of several three-dimensional crack propagation examples and comparisons with experiments.

Convergence study of crack-growth using the X-FEM. **Markus Peters** (Ruhr-Universität Bochum, Germany), Klaus Hackl (Ruhr-Universität Bochum, Germany) GA/CT1969/003

The eXtended Finite Element Method (XFEM) is a very efficient way to reduce mesh dependencies when analyzing crack growth. Displacements and stresses around the crack tip are calculated using additional shape functions which span the analytical displacement field around a crack tip.

Because of the fact that the extended shape-functions do not form a partition of unity in the transition elements, the crack path depends on

1. the number of elements used in the XFEM computation
2. the number of layers which are enriched by the crack tip functions and
3. the shape functions which are used for the standard FE

term.

We want to compare the crack-path for the crack-growth criteria (i) maximum hoop stress (ii) minimum of potential energy (iii) maximum of directional derivative of energy release using different configurations for the parameters in items 1., 2. and 3. and analyze the differences of the displacements and stresses obtained in the initial state.

Numerical determination of fatigue-crack growth in isotropic and anisotropic materials. **Markus Fulland** (Universität Paderborn, Germany), Martin Steigemann (Universität Kassel, Germany), Hans Richard (Universität Paderborn, Germany), Maria Specovius-Neugebauer (Universität Kassel, Germany) GA/CT1555/003

For the determination of fatigue crack growth in a three-dimensional structure basically two important questions do arise: Which path does the crack take? What is the crack growth rate and thus the remaining lifetime? In order to answer both questions usually the evaluation of the stress intensity factors K_I, K_{II} and K_{III} is necessary, since most 3D fracture criteria as well as the crack growth rate relations rely on those parameters. A very efficient way to numerically calculate the stress intensities on the basis of a 3D-FE-calculation is to first of all determine the energy release rates with the modified virtual crack closure integral method (MVCCI):

$$
\begin{aligned}
G_I(a,\Delta t_k)_k &= \tfrac{1}{\Delta t_k \Delta a} W_k^{\mathcal{Y}}, & W_k^{\mathcal{Y}} &= \tfrac{1}{2}\left[F_{i,k}^{\mathcal{Y}}(a)\cdot \Delta u_{i-1,k}^{\mathcal{Y}}(a)\right]\\
G_{II}(a,\Delta t_k)_k &= \tfrac{1}{\Delta t_k \Delta a} W_k^{x}, & W_k^{x} &= \tfrac{1}{2}\left[F_{i,k}^{x}(a)\cdot \Delta u_{i-1,k}^{x}(a)\right]\\
G_{III}(a,\Delta t_k)_k &= \tfrac{1}{\Delta t_k \Delta a} W_k^{z}, & W_k^{z} &= \tfrac{1}{2}\left[F_{i,k}^{z}(a)\cdot \Delta u_{i-1,k}^{z}(a)\right].
\end{aligned}
$$

The major benefit of this approach is the fact, that only non-singular fields (nodal forces $F_{i,k}$ and displacements $\Delta u_{i-1,k}$) are needed, which minimizes the mesh refinement demands. Moreover this method is applicable also for the most general anisotropic and inhomogeneous case, since no material assumptions are made in the theory. In the isotropic case the energy release rates can easily be converted to stress intensities either under the assumption of plane stress or plane strain conditions. For orthotropic materials however this conversions is much more complicated, since the energy release rates and stress intensity factors for the different fracture modes are no longer uncoupled.

In this contribution the authors will discuss the numerical issues in the process of determining fatigue crack growth in isotropic and anisotropic materials. This includes the effective calculation of energy release rates and stress intensities as well as the application of reliable 3D-fracture criteria and lifetime estimation for 3D structures. The numerical examples given in the talk will be carried out with the program system ADAPCRACK3D developed at the Institute of Applied Mechanics at Universität Paderborn.

This contribution is based on investigations of the collaborative research center SFB/TR TRR30, which is kindly supported by the DFG.

On the influence of a kink's asymptotic field on crack propagation. **Henning Schütte** (Ruhr-Universität Bochum, Germany) GA/CT3116/003

The aim is to highlight the influence of the kink developing at the beginning of mixed-mode crack growth on the propagation behavior of the crack. Le & Schuette [1],[2] have shown that the variational principle of a body containing a crack results in the principle of maximum energy release rate incorporating the stress intensity factors of the kinked crack. Here the influence of the kink and the kinking angle, resulting in a singular field around the corner, on the crack growth resistance is analyzed. The generalized stress intensity factors at the kinks corner are computed with the help of a FEM strategy. The influence of these on the plastic energy dissipated at the kink is determined using a small scale yieling approach. The impact of these results on mixed-mode crack propagation are discussed.

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GA/CTS4772/03: Damage models and analysis.

Organiser: Christian Miehe (Universität Stuttgart, Germany)
Co-organiser: Wolfgang Müller (TU Berlin, Germany)
Co-organiser: Dietmar Klingbeil (BAM Berlin, Germany)

Thermal-shock investigation of the hybrid-forming process. **Andreas Schneidt** (Universität Paderborn, Germany), Rolf Mahnken (Universität Paderborn, Germany) GA/CT4025/003

In hybrid processes for gradient structures, inhomogeneous, cyclic thermal-mechanical stresses and strains lead to higher risks of failure of the forming die. The main topic of the presentation is the validation of the finite-element calculation for a tool-like sample under complex thermal mechanical loadings to predict the material behavior. To validate the simulated model thermal shock tests of component- or tool-like specimens of the forming die are chosen. To obtain a sufficient amount of data, optical measuring systems are used to gain data for comparison of experiment and simulation. In this way model validation can be done on the basis of shapeŰ and strain-measurements. To analyze the damage, measurements using the current eddy method are done on the surface of the cyclic-thermal-shocked test specimen. The experimental damage analyzes of the thermal-shock tests, which are executed close to reality, are necessary to receive live-time dependent data for the influence of the thermal-mechanical loadings of the hybrid deformation process of the forming die.

Non-local modeling of thermomechanical localization in metals. **Arnd Flatten** (BAM Berlin, Germany), Dietmar Klingbeil (BAM Berlin, Germany), Bob Svendsen (Universität Dortmund, Germany) GA/CT2430/003

The modeling of dynamic, high-speed loading of metallic materials, encountered for example in crash or drop tests, as well as in high-speed forming and cutting processes, involves in general a number of processes and effects such as high strain-rates, hardening behaviour, heating due to mechanical dissipation, friction and contact, thermal softening, damage, deformation localization and shear-band development. In particular, the latter process represents an instability of the original uniform deformation field due to inhomogeneous material behaviour and/or geometrical effects, resulting in extreme grain stretching over a finite, narrow domain in the structure. Rate-dependent '*local*' models according to Johnson & Cook do not generally result in a physically correct shear-band development; e.g., involving a finite, non-vanishing shear-band thickness.

In the current work, an extension of such local models is presented as based on a corresponding extension of the *rate-dependence* of the material behaviour to one on the gradient

of the accumulated inelastic deformation *rate* for high-speed processes. In particular, attention is focussed on the intrinsic length-scales incorporated via the rate-dependency of these models. On this basis, we compare and contrast local and non-local approaches in the context of their application to the modeling and simulation of dynamic, adiabatic shear-banding in the alloy Inconel 718.

Work-roll surface degradation due to spalling of the oxide layer. **Wenge Zhang** (TU München, Germany), Christian Krempaszky (TU München, Germany), Ewald Werner (TU München, Germany) GA/CT3272/003

The rolled-in scale of hot-rolled steel sheets due to the surface degradation of the work rolls often cannot be tolerated for automotive applications. In hot rolling, the degradation of the work rolls has been related to several mechanisms: thermal fatigue of the roll surface due to temperature cycles undergone by the outer layers, fatigue of the surface layers due to cyclic mechanical stresses, abrasion of the roll surface due to the contact in the roll gap and breakdown of the work-roll surface. Breakdown of small surface particles is the coming source of rolled-in-scale. This breakdown process can be considered as following: an initiation of interface decohesion between the oxide layer and substrate material due to inhomogeneous of the oxide forming process, the propagation of these decohesion (or cracks) as a sequent of micro-buckling of the oxide film and finally the occurrence of micro spalling.

In this work we analyse the damage (often caused by the oxide layer spalling) evolution to a protective oxide layer on the roll surface and investigate the role of residual stresses in the oxide layer under the cyclic thermal loading during the micro-buckling. A theoretical estimation is made of the critical stress for the micro-buckling of oxide layer. The dependence of the spalling behaviour on the temperature and thickness of the oxide layer is determined by adopting the Hutchinson-Suo bi-material model. These results are helpful to determine the optimum operating parameters for the work roll and to reduce the downtime of the rolling equipment.

GA/CTS4769/03: Analytical and numerical methods (BEM).

Organiser: Wolfgang Müller (TU Berlin, Germany)
Co-organiser: Dietmar Klingbeil (BAM Berlin, Germany)

On the peculiarities of a crack growth path in an anisotropic solid. **Efim Shifrin** (Russian Academy of Sciences, Moscow), Robert Goldstein (Lomonosov Moscow State University, Russian Federation) GA/CT1987/003

A linear elastic problem for a straight crack, located on a symmetry axis of an orthotropic plane is considered. It is supposed that normal loads are applied at the infinity. The strength properties of the solid are supposed isotropic. It is shown that an ideal cut is not an appropriate model for a crack when a problem of a crack growth direction is considered. In this connection an elongated elliptical hole is considered as a crack model and maximal tensile stresses as a crack growth criterion. It is shown that for some class of orthotropic materials a crack deviates from the straight path just after it starts to grow. The problem of the stability of a straight crack path under Mode I loading is considered also. It is shown that for some class of orthotropic materials a straight crack path is unstable even in the conditions of uniaxial normal tension.

Computation of stress-intensity factors in a plane homogeneous anisotropic solid. **Martin Steigemann** (Universität Kassel, Germany), Markus Fulland (Universität Paderborn, Germany), Hans Richard (Universität Paderborn, Germany), Maria Specovius-Neugebauer (Universität Kassel, Germany) GA/CT1666/003

One of the main problems in Fracture Mechanics is the propagation of cracks in solids. There are various criterions for predicting crack paths but often the stress intensity factors K play an essential role. Let Ω a bounded domain in the plane with a selvage crack. Applying an external load p, the stress intensity factors K at the crack tip can be computed with the help of special solutions to the pure homogeneous Neumann problem of 2-dimensional elasticity theory

$$\nabla \cdot \sigma(\zeta) = 0\,, \quad x \in \Omega\,, \qquad \sigma^{(n)}(\zeta) = 0\,, \quad x \in \partial\Omega\,,$$

with singular behavior near the crack tip:

$$\zeta_{1/2}(x) = r^{-1/2}\Psi_{1/2}(\varphi) + \widetilde{\zeta}_{1/2}(x), \qquad r \to 0\,.$$

Namely,

$$K_{1/2} = \int_{\partial\Omega} p(x)\zeta_{1/2}(x)\,ds$$

$r^{-1/2}\Psi_{1/2}$ are eigenfunctions of the elasticity operator and can computed exactly for an isotropic, but only numerically for an anisotropic solid. $\widetilde{\zeta}$ is a solution with finite energy of the pure Neumann problem with nonhomogeneous data. Such a solution of the Neumann problem is only determined up to a rigid body motion and a solution u exists iff the body and boundary forces are self-balanced. A weak solution u of the pure Neumann problem exists and is unique by Korn's inequality and the Lax–Milgram-Lemma in the subspace

$$H^1_R(\Omega) = \left\{ u \in H^1(\Omega) : \int_\Omega u\,dx = 0, \int_\Omega \mathrm{rot}(u)\,dx = 0 \right\}$$

with $\mathrm{rot}(u) := \partial_{x_1} u_2 - \partial_{x_2} u_1$. This unique solution can be found by applying the projection

$$P_R : \quad H^1(\Omega) \longrightarrow H^1_R(\Omega)$$

defined by

$$P_R u := u - \frac{1}{|\Omega|}\int_\Omega u\,dx + \frac{1}{2|\Omega|}\int_\Omega \mathrm{rot}(u)\,dx \left(\begin{pmatrix} x_2 \\ -x_1 \end{pmatrix} - \frac{1}{|\Omega|}\int_\Omega \begin{pmatrix} x_2 \\ -x_1 \end{pmatrix} dx \right)$$

to an arbitrary solution u of the Neumann problem. For any solid, the functions $\widetilde{\zeta}$ can only computed numerically, for example, with the finite element method. The direct Galerkin discretization of the Neumann problem leads to a linear system of equations

$$\mathbf{A}\mathbf{u} = \mathbf{f}$$

for the discrete solution $\mathbf{u}$ with a positive semi-definite stiffness matrix $\mathbf{A}$ with three-dimensional kernel. A solution only exists, iff the source term $\mathbf{f}$ is orthogonal to this kernel. With the Krylov subspace method MinRes this system of equations can be solved and gives some discrete solution $\mathbf{u}$. Applying the discrete analogon $\mathbf{P}$ of P_R, the discrete solution $\mathbf{Pu}$ is the approximation of the unique normalized solution $u \in H^1_R(\Omega)$.

In our talk we will present numerical results for isotropic and in particular anisotropic solids. On different test specimens well-known in Fracture Mechanics we will show the accuracy of the weight function method and the advantages of projections when computing the pure Neumann problem numerically.

Acknowledgement: This contribution is based on investigations of the collaborative research center SFB/TR TRR 30, which is kindly supported by the DFG.

A BE-based finite element for crack propagation processes. **Bastian Helldörfer** (Universität Erlangen–Nürnberg, Germany), Günther Kuhn (Universität Erlangen–Nürnberg, Germany) GA/CT2570/003

A boundary element based crack propagation module for finite element systems within the framework of linear elastic fracture mechanics is presented.

When dealing with the simulation of 3D fatigue crack growth a series of problems has to be resolved. The long computing time resulting from the incremental algorithm which is needed because of the nonlinear nature of crack growth must be reduced. The singular stress field in the vicinity of the crack has to be captured adequately by the simulation method. Finally, after evaluating a valid 3D crack growth criteria and determining the new crack front, the new crack geometry must be integrated into the simulation model which is still a challenging task for arbitrary 3D crack front shapes.

In this talk a combined FEM/BEM simulation is proposed to overcome the mentioned problems. While the major part of the structure is meshed with finite elements only a small domain around the crack is modelled with boundary elements. These boundary elements define a finite macro element, for which a stiffness formulation is obtained by applying the Symmetric Galerkin Boundary Element Method. While the application of the FEM reduces the computational costs all fracture mechanical investigations are treated within the BEM which is advantageously here. Since displacements and tractions are only approximated on the boundary or on the FEM/BEM interface, no additional error resulting from the discretization is made in the interior of the BE domain and hence the stress singularity along the crack front can be captured properly. Based on the interior stress field reliable fracture mechanical parameters are obtained and after evaluating a valid 3D crack growth criteria a new crack geometry is determined. When updating the simulation model, only the surface oriented, BE based finite macro element is modified which is less complicated compared to volume oriented techniques.

Examples display the benefits of the proposed simulation technique.

Bridged interface cracks under transient thermal loading. **Mikhail Perelmuter** (Russian Academy of Sciences, Moscow) GA/CT721/003

To analyze of the stress-strain state and fracture parameters of fibers reinforced composites with bridged interface cracks under transient thermal and mechanical loading the direct boundary integral equations method (DBIEM) is used. The bridged zones of cracks are considered as parts of these cracks and it is supposed that nonlinear distributed spring-like bonds with given bond deformation law link the cracks surfaces. The bonds stresses are considered as the distributed tractions applied to the cracks surfaces at the bridged zone. It is supposed that these tractions depend on the crack surfaces displacements. The bridged zones sizes and theirs evolution depend on the type and structure of the matrix and fibers materials and transient external loading. The first step of the problem analysis is the solution of the thermal problem. Time stepping convolution formulation is used for solution of transient heat conduction problems. The results of the thermal problems solution are used as the initial data for the thermal stress problems. The DBIEM formulation based on the transient quasi-static uncoupled thermoelasticity is used for thermal stress problems solution. Modeling of the bridged interface cracks is based on the multi-domain DBIEM formulation. In the frames of this approach, the DBIEM equations for each homogeneous sub-region of the structure with addition boundary conditions along the interface boundaries and along the bridged zone of crack are considered. For general case of the nonlinear bonds deformation law the iterative procedure of the solution of the DBIEM equations is used. At the first step of this procedure is supposed that the bond stiffness has a constant value along of the whole bridge zone. Some results for the structures of a finite size containing material junction of different kind and shape with variation of bridged zone size and fibers property are presented. The comparison of the DBIEM results with the results obtained previously using singular integral-differential equations (Goldstein R.V., Perelmuter M.N. Modeling of bonding at the interface crack, Internal J. of Fracture, vol. 99, N 1-2, pp.53-79, 1999) is performed. The numerical analysis of the interface crack leads to a classification of the possible regimes of the interface cracks growth in dependence on the parameters of the bond deformation law and the transient thermal loading. This research was supported by Russian Foundation for the Basic Research, the number of the grants are 05-01-00191 and 05-08-18207.

Semi-analytical modelling of cracks with interacting faces in isotropic materials under harmonic load. **Oleksandr Menshykov** (University of Aberdeen, UK), Igor Guz (University of Aberdeen, UK) GA/CT837/003

In structural materials the existing cracks often have a non-zero initial opening or a complex shape. Under the consequent dynamic loading the opposite crack faces move with respect to each other and interact. The contact interaction results in the appearance of the contact forces in the contact region and changes significantly the stress and strain distribution near the crack tips. The shape of the contact region will change in time and must be determined as a part of solution. The complexity of the problem is further compounded by the fact that the contact behaviour is very sensitive to the materials of two contacting surfaces and the type of the external loading. Such dependences make the contact problem for crack faces highly non-linear. As the consequence, in the majority of studies the interaction of crack faces was neglected and, therefore, the real stress-strain distribution was ignored due to the difficulties of finding the appropriate solution.

The present work is devoted to the investigation of the contact interaction of the faces of a crack located in the homogeneous, isotropic, linear elastic 3-D medium under harmonic loading. The Signorini contact constraints are imposed and the friction is governed by the Coulomb law.

The problem is solved by the method of the boundary integral equations with the use of the iterative procedure. The solution is refined during the iteration process until the distribution of physical values satisfy the contact constraints. The contact forces and displacement discontinuity on the crack surface are investigated for different wave parameters (frequency, direction, etc) and different values of the friction coefficient. The effect of the parameters on the stress intensity factors is studied. The results are compared with those obtained without allowance for the contact interaction. The significant difference between compared results confirms the crucial importance of taking the crack faces contact interaction into account.

04, Minisymposia

GA/MP397/004: Experimental methods in structural dynamics.

Organiser: Dieter Weichert (RWTH Aachen, Germany)
Co-organiser: Fabrice Bremand (Université de Poitiers, France)

The tremendous progress in theoretical modelling and numerical simulation in mechanics over the last decades makes it increasingly important to validate highly sophisticated simulation models by adequate and pertinent experiments in order to avoid danger to produce apparently correct results with fallacious models by pure parameter adjustment. This however requires that experiments must reach the same degree of precision as results produced by numerical simulations. As a consequence, efforts to be put into experimental equipment and design and interpretation of experiments are also increasingly high. For this reason, many researchers give up to make experiences and concentrate exclusively on theoretical and numerical work. This mini-symposium advocates experimental mechanics as a necessary and important branch of research in mechanics going beyond the up-mentioned question of validation: Very often physical effects turn out to play a dominant role in experiments, that have not been adequately considered in theoretical and numerical modelling. Therefore, experiments frequently open ways for re-thinking modelling. This mini-symposium covers only a small part of experimental mechanics. The particular area this mini-symposium focuses on is the dynamic behaviour of structures and structural elements, especially under impulsive loading. Among others, the questions addressed are how to design adequately experimental set-ups, how to apply loads in a controlled manner, how to monitor and document the evolution of significant field quantities of the considered specimen in the dynamic process.

Experimental and numerical investigation of shock wave-loaded plates. **Marcus Stoffel** (RWTH Aachen, Germany), Ruediger Schmidt (RWTH Aachen, Germany), Dieter Weichert (RWTH Aachen, Germany) GA/MT3549/004

If thin-walled structures like plates or shells have to be designed as protection against blast loadings such as explosions, numerical simulations can turn out to be very helpful means for dimensioning. The large variety of commercial finite element codes based on different mechanical models, may however lead to quite different results in numerical application. It is therefore important to develope experimental techniques allowing to examine very precisely structural deformations under shock wave-loading conditions, which may be used in the assessment of numerical models. In the present study an experimental set-up for such purposes is presented. Two shock tubes are used to load circular metal plates by pressure waves, causing high strain rate deformations that lead to inelastic deformations up to rupture. The plates can be loaded repeatedly and alternately from both sides. In order to record displacements and deformed shapes, a short time measurement technique developed in recent years is applied, consisting of capacitive displacement sensors and piezoelectric pressure sensors suitable to record signals during the impulse period in the range of several microseconds.Parallely, numerical simulations are carried out, using different viscoplastic constitutive equations and damage laws. In order to determine the elastic, hardening and viscous parameters of the considered materials, tension tests at different strain rates are carried out seperately. The damage parameters are identified by the change of elastic stiffness in cyclic tension tests.

Advanced instrumentation for dynamic material testing. **Stefan Hiermaier** (Ernst-Mach-Institute, Germany), Frank Huberth (Ernst-Mach-Institute, Germany), Thomas Meenken (Ernst-Mach-Institute, Germany) GA/MT3552/004

Predictive capability of numerical methods in computational mechanics means the ability to predict structural response under varying loading conditions, change of geometries and variations in boundary conditions without adaptation of material parameters. Only with that capability approved, numerical simulation can be treated as a useful tool in engineering design.
In order to meet the mentioned demanding to a predictive tool, the mathematical model describing the material behaviour has to cover all relevant characteristics in the physical behaviour of the modelled material. Additionally, the free parameters in the model need to be derived from precise material tests under well defined stress and strain states. The latter, a precisely known combination of stresses and strains in the sample, is what distinguishes a material test from a component or validation test.
Therefore, it is of primary importance for material characterization to guarantee the assumed stress and strain states in a test set-up or to take changes into consideration if necessary. A more complex the material behaviour and the more dynamic the loading situation, the harder it gets to guarantee these demands. That is why material tests under high strain rate conditions need additional attention. Wave propagation effects cause transient stress-strain states.
Two specific topics will be covered in this paper. One concerns the non-constant volume under plastic deformation of some polymers. Test set-ups and enhanced qualities of multi-directional optical strain measurement with regard to volume change will be proposed along with the related additional modelling efforts. Secondly, the special case of testing low impedance materials under high strain rates in the range of $10^2\ 1/s$ to $10^3\ 1/s$ will be introduced as an example to identify the admissible phases in the testing.

Identification of the shoulder joint centre. **Tony Monnet** (Université de Poitiers, France), Claude Vallée (Université de Poitiers, France), Kossi Atchonouglo (Université de Poitiers, France) GA/MT3870/004

The analysis of joint forces and moments underlying human movement has typically been based on inverse dynamics. Poor estimations of the joint centre locations have led to the distortion of computed angles and moments. Joints centres can be estimated using a predictive or a functional approach. The main sources of error of the predictive approach are: marker location, regression uncertainty and anthropometric measurement. The functional approach is affected by the presence of noise. In this paper we propose a functional method requires only position of markers in proximal and distal segments. The joint centre is then localized as the point belonging both segments by solving a linear system. The method is applied for two different movements. Results are the same for the two movements and are very reproductible.

Out-of-plane displacement measurement near the crack tip during a crack propagation: validation of a 3D formulation for a specimen in PMMA loaded in mode I. **Fabrice Bremand** (Université de Poitiers, France), Stephen Hedan (Université de Poitiers, France), Valery Valle (Université de Poitiers, France), Mario Cottron (Université de Poitiers, France) GA/MT3872/004

This paper proposes to validate experimentally a 3D formulation of the out-of-plane displacement at the vicinity of the crack tip during crack propagation for specimens loaded in mode I. For that the experimental data of the out-of-plane displacement near the crack tip is made using a Michelson interferometer. This technique allows determining the relief variations of a few microns. With the obtained interferograms, we can extract the phase (thus the relief) by using a new numerical approach based on the principle of images correlation between real fringes and virtual fringes. Two tests were realized in the PMMA specimens loaded in mode I with the same loading and the same crack propagation velocity. We compare the experimental results with the 2D theory of Westergaard in plane stress hypothesis and a proposed 3D formulation. This one was given for specimens loaded in mode I and for static cracks. It is function only of 3D effects related to Poisson's effect. However in dynamic, the transient effects appear and are related to the crack propagation velocity. The 3D effects and transient effects lead to results equivalent to experimental ones in terms of displacement but are completely different to results given by the 2D theory near the crack tip. From experimental results, an optimisation process is performed to get the three constants defining the 3D formulation as well in static as in dynamics. We note that these three parameters are equal for two tests. We can show that these three constants are independent of the crack length, and of the dynamic stress intensity factor. In conclusion, a Michelson interferometer associated to a numerical analysing technique for a single image is powerful tool for the relief study near the crack tip during crack propagation. The 3D formulation, we proposed in static, can be extended in dynamic studies by taking into consideration the 3D and transient effects during crack propagation.

04, Short Communications

GA/CTS4537/04: Non-classical applications.

Organiser: Holm Altenbach (Universität Halle–Wittenberg, Germany)
Co-organiser: Friedrich Gruttmann (TU Darmstadt, Germany)

On buckling of carbon nano-tubes. **Grzegorz Litak** (Technical University of Lublin, Poland), Alois Steindl (TU Wien, Austria), Hans Troger (TU Wien, Austria) GA/CT1266/004

We investigate a single walled Carbon Nanotube under an axially-directed compressive line loading applied at both of its edges. The expected buckling behavior we study by application of a molecular computation approach ([1]). We formulate a global potential and search for its minimum to obtain the equilibrium configuration. Using besides the main parameter, which is the value of the loading, as second parameter the diameter of the tube, we are able to define the critical value of the diameter, for which we obtain the coincident case of Euler and local shell buckling.

[1] Proykova A., Iliev H.,2004, *Simulated Stress and Stretch of Single Walled Carbon Nanotubes.* Proceedings of SIMS 2004 Copenhagen, Denmark (Eds. B.Elmegaard, J.Sporring, K.Erleben, K.Sorensen)

The stability of a pre-stressed annular thin film in tension. **Ciprian Coman** (University of Glasgow, UK) GA/CT2749/004

Asymptotic properties of the neutral stability curves for a linear boundary eigenvalue problem which models the wrinkling instabilities of an annular thin film in tension are considered. The film is subjected to imposed radial displacement fields on its inner and outer boundaries and, when these forces are sufficiently large, the film is susceptible to a wrinkling instability. The critical values at which this onset occurs are dictated by the solution of a fourth-order ordinary differential eigensystem whose eigenvalue λ is a function of $\mu\,(\gg 1)$, a quantity inversely proportional to the bending stiffness of the plate, and n, the number of wrinkles that occur around the film. Previous numerical studies have provided information as to the form of $\lambda(\mu, n)$ but, by their very nature, these are unable to address certain important questions concerning the preferred instability mode or the size of imposed displacement field necessary to induce wrinkling in the thin-film limit. Here WKB and boundary-layer asymptotic methods are used to examine these issues and comparisons with direct numerical simulations made.

this is joint work with Andrew P. Bassom (University of Western Australia). The financial support from The Carnegie Trust for the Universities of Scotland, and from the University of Glasgow are gratefully acknowledged.

[1] C.D. Coman and A.P. Bassom; On the neutral stability curves of a pre-stressed annular thin film in tension. Preprint 2006.
[2] C.D. Coman and D.M. Haughton; Localised wrinkling instabilities in radially stretched annular thin films. Acta Mechanica 185, pp.179–200 (2006).
[3] C.D. Coman; On the applicability of tension field theory to a wrinkling instability problem. Acta Mechanica (to appear).

Numerical analysis of telephone-cord buckling mode delamination of compressed thin films. **Viet Dung Pham** (Institut für Werkstoffe und Mechanik im Bauwesen„ Germany), Friedrich Gruttmann (TU Darmstadt, Germany) GA/CT2970/004

Experiments of equi-biaxial compressed thin films on substrates provide different forms of delaminations. In Reference [1] the authors perform measurements on compressed diamond-like carbon films (DLC) on nominally flat glass substrates to characterize the various forms of blisters. Straight-sided buckles are rarely observed. In contrast to that the so-called telephone cord delamination occurs in many systems with applied high residual stress levels.

In the presentation we consider the equi-biaxial compressed thin films on rigid substrates. Since small geometrical imperfections are used to initiate buckling. A 5-parameter Reissner-Mindlin shell model for thin films is used, where the interface between film and substrate is chosen as the reference surface. The used 8-noded interface element is compatible with the 4-noded shell element. For the interface we postulate the existence of a cohesive free energy as a function of the opening displacement vector and internal variables. For the irreversible delamination process we use a cohesive law either of a exponential type with constant given parameters or of a bi-linear type, where parameters depend on the combination of modes I, II and III. In order to model the large delamination exactly we use the energy criterion of the steady-state growth.

[1] M.W. Moon, H.M. Jensen, J.W. Hutchinson, K.H. Oh, A.G. Evans; The characterization of telephone cord buckling of compressed thin films on substrates, J. Mech. Phys. Solids, 50, 2355–2377, 2002.

[2] F. Gruttmann, V.D. Pham; A finite element model for analysis of buckling driven delaminations of thin films on rigid substrates, in preparation.

Comparative analysis of description of elastic plane waves by Murnaghan and Signorini nonlinear models. **Jeremiah Rushchitsky** (Timoshenko Institute, Kyiv, Ukraine), Carlo Cattani (Università degli Studi di Salerno, Italy) GA/CT2225/012

An attempt is realized to outline in the chronological ordering the development of theory of elastic nonlinear waves in materials, where five stages are emphasized. Further the attention is concentrated on distinctions and similarities in the analytical description of propagation of plane polarized hyperelastic waves within the assumption that nonlinear deformation of material takes place by the Murnaghan and Signorini models, as well as in matching the fundamentals of propagation the mentioned waves when waves are described by theories based on distinct enough Murnaghan and Signorini potentials. For the family of fibrous composite materials with micro- or nanofibres, a computer simulation of evolution of initial harmonic profiles is studied. A few short movies on distinct scenarios of evolution will be presented.

A contribution to the modelling of metal foams on the mesoscale. **Daniel Schwarzer** (Universität Karlsruhe, Germany), Sébastien Gatouillat (Universität Karlsruhe, Germany), Carsten Proppe (Universität Karlsruhe, Germany) GA/CT1890/004

Due to their useful properties in lightweight construction and due to their excellent behaviour in energy absorption for example in crash mechanics, metal foams became an interesting and in literatur often examined material. In this talk, the focus of the investigations lies on the mechanical properties of mainly metal foams and their modelling on the mesoscale. Starting with the examinations of analytical models based on Gibson and Ashby [1], different extensions of these models are taken into account and their influence on the mechanical properties are dicussed and compared. The goal of this contribution is to find a model, which shows the important effects of the foam on the mesoscale, but stays simple enough to be useful in further investigations in multiscale modelling of foams.

[1] Gibson, L.J. and Ashby, M.F.; *Cellular solids – Structure and properties*, 2nd edition. Cambridge University Press, Cambridge, 1997.

Damping of structural vibrations using an electromotive eddy current damper. **Siewert Christian** (Universität Hannover, Germany), Lars Panning (Leibniz Universität Hannover, Germany), Christoph Gerber (ALSTOM, Schweiz, Switzerland), Andreas Hohl (Universität Hannover, Germany), Buerge Annika (Universität Hannover, Germany) GA/CT2404/004

Structural vibrations are normally the cause for high cycle fatigue failure (HCF) in technical structures. For example, the blades of rotating bladed turbine disks are subjected to fluctuating gas forces during operation that cause blade vibrations. One of the main tasks in the design of turbomachinery blading is the reduction of the vibration amplitudes of the blades to avoid high resonance stresses that can cause a HCF blade damage. It is well known that the vibration amplitudes of the blades can be reduced significantly to a reasonable amount by means of friction damping devices such as underplatform dampers, tip shrouds and damping wires.

If the temperature of the working fluid is not excessively high, the use of an electromotive eddy current damper can be a possible alternative to this well known classical friction damping devices. If a conducting material is moving in a stationary magnetic field, eddy currents are generated inside the conductor. These eddy currents cause an energy dissipation effect, therefore a damping effect is generated. This damping effect can be used to reduce the resonance amplitudes and therefore to decrease the risk of a HCF failure. In contrast to classical friction damping devices, the eigenfrequencies of the structure are not affected by the use of an electromotive eddy current damper.

In this paper, the electromotive eddy current damper model presented in [1] is extended. The modified model is validated by comparing measured and simulated data for a beam model. It is shown that the measurements and the simulation results are in good agreement. Furthermore, the electromotive eddy current damper is applied to a turbine blading with shroud and snubber coupling. The results are compared to the results computed with classical friction damping devices with respect to the influence on the vibration amplitude and resonance frequency of a steam turbine blading.

[1] H. A. Sodano, J. S. Bae, D. J. Inman, W. K. Belvin: *Improved Concept and Model of Eddy Current Damper*, Transactions of the ASME, Vol. 128, 2006

GA/CTS4538/04: Stability and dynamical problems.

Organiser: Dietmar Gross (TU Darmstadt, Germany)
Co-organiser: Friedrich Gruttmann (TU Darmstadt, Germany)
Co-organiser: Holm Altenbach (Universität Halle-Wittenberg, Germany)

Stability analysis of large flexible, earth-orbiting structures. **Wolfgang Steiner** (FH Oberösterreich, Austria) GA/CT1120/004

Large flexible structures could be one of the most challenging space technologies of the future. A well known example is the *space elevator* enabling astronauts to climb up a 36000km long tether leading to a geostationary orbit. In general we could consider an arbitrary flexible structure in a stationary circular motion around the earth or another celestial body.

Usually such systems require two problems to be solved: the strength of the materials and an overall stability analysis. The latter one is a non-trivial task since in orbiting systems not the angular rate but the angular momentum must be kept constant when applying for example Dirichlet's criterion. In particular, this fact becomes important, if the system's dimension is in the magnitude of the orbital radius. Therefore, this presentation will focus on a general applicable method to discuss the stability of flexible earth orbiting structures.

The analysis process bases on the *reduced energy momentum method* by J.C. Simo, T.A. Posbergh and J.E. Marsden, which has been specialized to systems with cyclic coordinates by the author. In the presented approach the second variation of an *amended potential* is derived from the system's equilibrium configuration, which is obtained from a standard Finite Element Analysis with common solvers such as ABAQUS. A practical example will be discussed to demonstrate an application of the method.

Basic studies on the dynamics of rotating circular structures. **Maik Brinkmeier** (Universität Hannover, Germany), Udo Nackenhorst (Leibniz Universität Hannover, Germany) GA/CT2147/004

In this presentation the dynamic effects due to rotation on spinning circular structures will be discussed by analytical, experimental and numerical investigations. Basic phenomena of spinning are studied on the analytical solution of a spinning ring. The observed effects will be underlined by rather simple experimental investigations on a rotating wine glass. Based on this fundamental knowledge special attention has to be payed to the finite element modeling and implementation of

the eigenvalue analysis of gyroscopic systems, which requires the numerical solution in complex numbers. Besides the influence of rotational speed, the disturbances due to rolling contact will be discussed on rotating tubes as well as detailed finite element models of rolling tires. The application of these techniques with emphasis to the prediction of tire noise will be outlined.

Nonlinear dynamics of an inclined cable subjected to boundary motion conditions. **Anna Woszczyna** (Wroclaw University of Technology, Poland), Danuta Bryja (Wroclaw University of Technology, Poland), Dawid Prokopowicz (Wroclaw University of Technology, Poland) GA/CT2210/004

The paper is devoted to the dynamic modelling of an inclined cable being an element of suspended structures such as cable-stayed bridges, suspension bridges, suspended pipelines [1,2]. Spatial cable vibrations are considered from the viewpoint of kinematic excitation caused by a motion of connecting points between the cable and suspended structure or pylon. Basing on equilibrium state analysis of a differental cable element in deformed configuration, the nonlinear equations describing in-plane and out-of-plane cable vibrations are derived. The final general form of the equations is obtained by applying the standard Galerkin's procedure. General equations are adjusted to the particular types of cable geometry distinguished by a small or large sag-to-span ratio and horizontal, vertical or inclined cable chord. The proposed cable model is formulated so as to be useful for analyzing suspended structures by substructure approach [3]. Examples of numerical studies: vibrations of planarly suspended beam and spatially suspended pipeline are presented for invesitigating the nonlinear behaviour of structures.

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Non-linear vibrations of a ropeway system with moving passenger cabins. **Marta Knawa** (Wroclaw University of Technology, Poland), Danuta Bryja (Wroclaw University of Technology, Poland) GA/CT2235/004

The dynamic model of a carrying rope for a bicable aerial ropeway is formulated. The cable is anchored at one end point of the multi-span track and tensed by the counterweight at the other end point. Dynamic behavior of the carrying rope is considered independently from the hauling rope [1]. To describe non-linear in-plane vibrations excited by moving masses of passenger cabins a closed form model with a Green-Lagrange relative strain is adopted. The equations of motion of the system are derived on the basis of Lagrangian's equations with a Ritz approximation of cable displacement is applied [2]. Numerical simulations of the dynamic response of the system are presented for investigating the non-linear behavior of the cable.

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Radiation problem of normal stress-loading of bore surface. **Arnold Snitser** (Vernadskiy Tavrichesky National University, Ukraine) GA/CT4309/012

We study the radiation of elastic waves which are generated by normal loading of a circular strip applied on the free surface of a cylindrical cavity in elastic medium and having a harmonic time-dependence. The stress and displacement field is represented by contour integrals. By using the saddle-point method stress and displacement asymptotic expansions in the far field were obtained. It is shown that in the far field P-waves bring radial displacements and stresses, and perpendicular to these, displacements and stresses are caused by SV-waves.

As a result the relative distribution of wave-energy radiation in accord to type of waves (P-, S- and Biot surface waves) and its dependence on vibrator's frequency, relative diameter of the hole and width of circular strip loading were obtained. In the paper orientation diagrams of radiation of elastic P- and S-waves and their dependencies on frequency and geometrical parameters are presented too.

Stochastic FEM with local polynomial-chaos approximations. **Carsten Proppe** (Universität Karlsruhe, Germany) GA/CT2125/004

Polynomial-chaos expansions of response quantities have been widely used in Computational Stochastic Mechanics and are well documented. Introduced in conjunction with a truncated Karhunen-Loève-representation of the input random field, they represent global approximations in the Hilbert space of functions of (usually standard Gaussian) random variables. However, the global approximation character may lead to inefficient convergence behavior for higher order response moments or small response probabilities. This has been pointed out recently in [1]. Therefore, after the multiplicative decomposition in deterministic and a random part, local polynomial expansions of the solution are introduced by partitioning the domain of random variables and the physical domain. By carefully choosing the local basis [2], the problem decouples in the random domain. The expansion coefficients can then be determined independently by parallel processing. Moreover, local expansions allow to construct new hybrid simulation schemes, that is, combinations of analytical and simulation based techniques. For reliability estimation, the expansion can be interpreted as a local response surface. Starting from the global approximation, a local response surface can be constructed by computing the design point and sensitivities. After that, suitable local approximations can be introduced by decomposing the region of most probable failure. [1] R. V. Field Jr., M. Grigoriu, "On the Accuracy of the Polynomial Chaos Approximation", Probabilistic Engineering Mechanics, v. 19, p. 65-80, 2004. [2] I. Babuska, R. Tempone, G. E. Zouraris, "Solving Elliptic Boundary Value Problems with Uncertain Coefficients by the Finite Element Method: The Stochastic Formulation", Computer Methods in Applied Mechanics and Engineering, v. 194, p. 1251-1294, 2005.

GA/CTS4536/04: Shells, plates and beams, II.

Organiser: Friedrich Gruttmann (TU Darmstadt, Germany)
Co-organiser: Holm Altenbach (Universität Halle-Wittenberg, Germany)

complex loading and loss of the stability of the cylindrical shell: experimental investigation. **Vladimir Fedenko** (Dnipropetrovs'k National University, Ukraine) GA/CT1690/004

The numerous experimental investigations, devoted to the behaviour of ma-terials at complex loading, showed that for the same stresses, but reached by the various paths, the strain states are various. This fact gives the foundation to assume that for complex loading paths effect of "loading history" on values of stability pa-rameters of thin-walled constructional element, working outside elasticity, is pos-sible.

Investigation of loss of stability and bearing capacity of smooth cylindrical shells made from an aluminum alloy was carried out by experimental methods. The shell slenderness ratio (the ration of shell radius to its thickness) was equal 23.6 and 26.2 and shell was loaded by axial compression and external hydrostatic pres-sure. The results were obtained for simple and complex loadings. The simple load-ing which was carried out in experiments, is represented in loading space by a ray with various slope, and the complex loading is realized in the same plane by two-segment lines in which the first loading segment is carried out by axial compres-sion, and second segment - by combined action of axial compression force and ex-ternal hydrostatic pressure. The angle of the break of loading path was chosen in the interval $[0,\pi/2]$, and the length of the first segment was chosen equal to $0.95P^*$, where P^* Ű critical parameter of compression force at simple load-ing.

Areas in which depending on shell slenderness ratio the complicated loading raises critical values of exterior loadings from 14% up to 23% are founded. It is experimentally shown, that the phenomenon of raise of bearing capacity of a shell is expression of deformation anisotropy which is "induced" in a material of a shell as a result of prior complex loading.

The influence of semi-rigid connections on the shakedown of elasto-plastic frames. **Sandor Kaliszky** (Budapest University of Technology and Economics, Hungary) GA/CT1078/004

The main structural elements of steel framed multi-storey structures are the columns, the beams and their connections. The assumption that the connections are either rigid or pinned has been widely applied in the past. The actual behavior of the connections is however somewhere between these limits and they are semi-rigid [1,2]. This circumstance can influence significantly the behavior of the structure therefore has to be taken into account in the analysis and design. The aim of this paper is to analyze the influence of the semi-rigid connections on the shakedown of elasto-plastic steel framed structures under multi-parameter static loading. In addition to the shakedown analysis, to control the plastic behavior of the structure, bound on the complementary strain energy of the residual forces is also applied [3]. The formulation of the problem yields to nonlinear mathematical programming which is solved by the use of sequential quadratic algorithm.

The results of the numerical calculation are in agreement with the expectation, that the stiffness of the semi-rigid connections can influence significantly the magnitude of the shakedown parameter. In the presented example the average change of this parameter 15–20%. However, this effect depends very much on the number of the semi-rigid connections, the arrangement of the structure and the loads, the ratio of the lengths of the beams and columns and several other circumstances. Therefore further investigations are necessary to make more general statements.

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A new approach to analysis of free beam vibrations. **Vasily Saurin** (Institute for Problems in Mechanics RAS, Russian Federation), Georgy Kostin (Institute for Problems in Mechanics RAS, Russian Federation) GA/CT808/004

Based on the linear theory of elasticity and the method of integrodifferential relations a countable system of ordinary differential equations is derived to describe 3D longitudinal, lateral, and torsional free vibrations of rectilinear beams. In the approach under consideration the stress-strain relation is specified by an integral equality instead of the local Hooke's law. After expansion of unknown stress and displacement functions in polynomial series with respect to transversal Cartesian coordinates and system decomposition due to domain symmetry the consistent boundary value problems are solved and the bilateral estimation criteria of solution errors are proposed in order to analyze the algorithm convergence rate. The influence of geometrical and elastic characteristics of rectilinear beams on eigenfrequencies and shapes is investigated. The various kinds of longitudinal, lateral, and torsional free motions are found out in the models under study.

The vibrational behaviour of bladed disks with multiple coupling devices. **Andreas Hohl** (Universität Hannover, Germany), Buerge Annika (Universität Hannover, Germany), Siewert Christian (Universität Hannover, Germany), Lars Panning (Leibniz Universität Hannover, Germany) GA/CT2480/004

In turbomachinery applications turbine blades are subjected to high static and dynamic loads. Static loads are due to centrifugal stresses and thermal strains. Especially the dynamic excitation caused by fluctuating gas forces results in high vibration amplitudes which can lead to high cycle fatigue failures (HCF). Therefore, in practical applications, coupling devices like underplatform dampers, lacing wires und tip shrouds are installed to the structure. In case of blade vibrations the relative displacements between these coupling devices and the blades generate friction forces. The resulting energy dissipation provides additional damping to the structure. Furthermore, coupling devices, in particular tip shrouds, snubbers and lacing wires, increase the stiffness of the structure. Hence, they lead to a shift of the resonance frequencies.

So far, only effects of single coupling devices and the influencing properties have been examined. Within this paper the effect of multiple couplings is determined and compared with single couplings. The forced response of multiple coupled turbine bladings is calculated under consideration of geometrical and mechanical parameters of the blading and contacts, respectively. The results are compared with the single coupled blading. Furhermore, different coupling devices like underplatform dampers, connecting pins and shrouds are compared with respect to their effectiveness. Especially the influence on the resonance frequency and the vibration amplitudes is analysed.

The results of the simulation is verified in measurements at a two-blade non-rotating test rig with an underplatform damper and connecting pins in different configurations.

Elastic–plastic states of a rotating inhomogeneously-heated strain-hardening hollow shaft. **Eray Arslan** (Middle East Technical University, Turkey), Ahmet Nedim Eraslan (Middle East Technical University, Turkey), Werner Mack (TU Wien, Austria) GA/CT1952/004

Structures like rotating heat pipes are loaded by mass forces as well as by radial temperature gradients. To optimally utilize the material, it is of interest not only to predict the onset of yield but also, since plastic deformation may be admitted under certain circumstances, to study the behaviour in the elastic-plastic range. While several investigations on either mechanically or thermally loaded hollow cylinders are available, a solution for combined loading by rotation and an inhomogeneous temperature distribution has not been given hitherto; due to the non-linearity inherent in elastoplasticity, it cannot be found by mere superposition. Hence, based on Tresca's yield condition and the flow rule associated with it, the distribution of stress, strain and displacement in a linearly strain hardening elastic-plastic hollow shaft subject to monotonously increasing angular speed and a positive radial temperature gradient is investigated. Presupposing circular symmetry and plane strain conditions, the problem is amenable to an analytical treatment. A main result is that depending on the temperature difference between the outer and inner surface qualitatively different types of solutions may occur, and that a moderate temperature difference on the one hand reduces the elastic limit angular speed but on the other hand increases the fully plastic angular speed as compared to the isothermal case.

GA/CTS4535/04: Shells, plates and beams, I.

Organiser: Reinhold Kienzler (Universität Bremen, Germany)
Co-organiser: Friedrich Gruttmann (TU Darmstadt, Germany)
Co-organiser: Holm Altenbach (Universität Halle-Wittenberg, Germany)

Numerical benchmarks for creep-damage modeling. **Holm Altenbach** (Universität Halle-Wittenberg, Germany), Yevgen Gorash (Kharkiv National University of Technology, Ukraine), Konstantin Naumenko (Universität Halle-Wittenberg, Germany) GA/CT2548/004

The aim of creep modeling is to reflect basis features of creep in structures including the development of inelastic deformations, relaxation and redistribution of stresses as well as the local reduction of material strength. A model should be able to account material deterioration processes in order to predict long term structural behavior and to analyze critical zones of creep failure. In recent years general purpose finite element codes have become the widely accepted tool for the structural analysis. To consider the creep and damage processes, a specific constitutive model with selected internal state variables, special types of stress and temperature functions as well as material constants identified from available experimental data should be incorporated into the commercial finite code by writing a user defined material subroutine. To assess the reliability of the developed subroutine as well as the accuracy of the results with respect to the mesh density, the time step, and iteration methods, numerical benchmark problems are required.

In this lecture we present several problems of creep-damage mechanics which can be solved by approximate analytical methods. The reference solutions will be compared with the finite element solutions by ANSYS and ABAQUS finite element codes with developed user subroutines.

Nonlinear deformation of cylindrical shells with variable parameters. **Olga Tumashova** (Lvivska Politechnica, Ukraine) GA/CT3285/004

The present paper is devoted to working out the effective approach to numerical research in geometrically nonlinear statement of stress-strained state of flexible shallow cylindrical panels of finite dimensions with variable hardness or variable curvature along the generatrix y and solving two-dimension nonlinear problem based on consecutive application of the methods of Vlasov-Kantorovich, methods of linearization and discrete orthogonalization. Consided the deformation of the elastic shallow cylindrical panel with variable thickness and curvature is under the influence of normal surface load q.

Elastic-plastic sandwich beams with optimized properties for the impact case. **Jürgen Schmidt** (Universität Erlangen-Nürnberg, Germany), Werner Winter (Universität Erlangen-Nürnberg, Germany), Günther Kuhn (Universität Erlangen-Nürnberg, Germany) GA/CT2898/004

The objective is to obtain plane lightweight structures having an optimal performance concerning impact loadings. For this purpose sandwich structures with solid faces and cellular cores exhibit suitable multifunctional characteristics which enclose high structural rigidity and distinct energy absorption. To determine optimal design the used criteria cover failure mechanisms that dissipate maximum energy and lead to minimum displacement in addition with minimum structural thickness and weight.

In this contribution sandwich beams consisting of stainless steel faces and aluminium foam cores are subjected to low velocity impact. The identified design variables are the top and bottom face thicknesses as well as the core thickness. The design approach for this test configuration is based on simulation results performed by an explicit finite element code. Experimental tests are carried out on cellular aluminium to fit the used material constitutive law. Limits of accuracy are revealed for this material model in which material inhomogeneities in the cellular metal are the main reason for scatter in test results. For the applied optimization method it is gone into details.

Optimization results are presented and discussed. Beyond that results are compared in experiment and simulation to assess the correlation.

Application of the conditional moments method to multi-layered anisotropic shells. **Wolfgang Müller** (TU Berlin, Germany), Ralf Wille (TU Berlin, Germany), Lidiia Nazarenko (TU Berlin, Germany) GA/CT2345/004

In the present paper the model of non-linear deformation of stochastic composites under elevated loading is applied for investigation of the stress-strain state of tires. The tire is described geometrically non-linear as a multi-layered anisotropic torus shell with low transfer shear stiffness. The layers are treated as rubber matrix strengthened by metal or cord fibres. The problem can be solved stepwise. At the first stage we determine the effective properties of each of the layers and of the whole tire by the method of conditional moment functions. This method is based on the solution of statistically non-linear equations of the mechanics of a deformable solid. Based on the analytical and numerical approach the algorithm for the determination of non-linear deformative properties of such a material is constructed. Then the stress-strain state of the tire is studied on the basis of equations of shell theory. In this case the tire is considered as a homogeneous shell with averaged properties. At the next stage local problems of tire mechanics can be solved by using the finite element method considering the real structure of the tire in the place of stresses concentration. Boundary conditions for the local problem can be formulated on the basis of the solution of the global one.

Investigation of orthotropic non-thin non-circular varying thickness cylindrical shells using B-splines. **Sergiy Yaremchenko** (National Academy of Sciences of Ukraine, Kyiv) GA/CT1864/004

Non-circular cylindrical shells made of inhomogeneous anisotropic materials are widely used for building of structure elements in modern engineering. The effective approach is presented to this class shells design. Elliptical and corrugated cross-section cylindrical shells of varying thickness with hard clamped butt-ends is under consideration. A material of shell is orthotropic. The Timoshenko theory is used for description stress-strained state of shells. It lets us to take into account shear deformation and to solve problems for non-thin shells.

Let s be coordinate in directrix and θ be angular parameter in generatrix direction. The decision functions are components of displacement vector u, v, w and complete turn angles ψ_s, ψ_θ. Resolving system consist of five equations with partial derivatives and may be represented as

$$\mathcal{L}\bar{N} + \bar{f} = 0$$

where $\bar{N} = \{u, v, w, \psi_s, \psi_\theta\}$, $\mathcal{L}$ is linear differential operator of second order, and $\bar{f}$ are functions that represent the loads. Adding boundary conditions to the system we obtain two-dimensional boundary problem. Sought quantities are represented as

$$u = \sum_{i=0}^{N} u_i(\theta)\varphi_i(s), v = \sum_{i=0}^{N} v_i(\theta)\varphi_i(s), w = \sum_{i=0}^{N} w_i(\theta)\varphi_i(s),$$
$$psi_s = \sum_{i=0}^{N} \psi_{si}(\theta)\varphi_i(s), \psi_\theta = \sum_{i=0}^{N} \psi_{\theta i}(\theta)\varphi_i(s), \quad (1)$$

where u_i, v_i, w_i, ψ_{si}, $\psi_{\theta i}$ are unknown functions and φ_i are linear B-splines combinations of third power, that satisfy boundary equations on the butt-ends. If we put these latter expressions into the main equation, and into boundary conditions on straight contours, and demand satisfaction at $N+1$ points of collocation, we obtain a one-dimensional boundary problem with system of ordinary differential equation of $10(N+1)$ order, which is solved by the stable numerical method of discrete ortogonalization.

GA/CTS4539/04: Analysis of the modelling error.

Organiser: Christian Miehe (Universität Stuttgart, Germany)
Co-organiser: Friedrich Gruttmann (TU Darmstadt, Germany)
Co-organiser: Holm Altenbach (Universität Halle–Wittenberg, Germany)

Model adaptivity and Green's functions. **Friedel Hartmann** (Universität Kassel, Germany) GA/CT3077/004

The reliability of computer predictions has become known as the subject of Verification and Validation (V&V). The verification process addresses the quality of the numerical results while the validation process addresses the quality of the model. Both problems center on the approximation of the Green's function of the governing equation. How accurate is the approximation of the Green's function and does the model approximate the correct Green's function? The numerical error as well as the modeling error strongly depend on the nature of the Green's functions, their rate of decay, their domain of influence and their shifts (Green's function are pseudo differential operators).

Things become additionally complicated in that structures are made of composite materials so that homogenization techniques tend to blur the picture and multi scale modelling complicates the resolution of the (numerical) Green's functions. We know that the error in a (linear) FE analysis is attributable to the error $G_0 - G_h$ in the Green's functions and to gain accuracy we must improve the projections G_h. Adaptive methods based an this duality technique have been applied very successfully in recent years. This technique is also the key to the assessment of the modelling error. Unlike standard error analysis where we study the numerical error $u - u_h$, we now focus also on the modelling error $u - u_0 + u_0 - u_0^h$ where u_0 is the exact solution of a simplified problem (after some homogenization techniques are applied) and u_0^h is its FE approximation. The issue are therefore techniques which allow to adaptively refine a model so that the sensitivity and reliability of the model can be 'guaranteed' with regard to a certain output value. The *a posteriori* error estimates required can be developed in the same framework as the now 'classical' duality approach of Rannacher [1]. We shall outline a general technique for comparing coarse and fine models and to produce error estimates for computing modelling errors.

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Energy-momentum conserving integration with AES elements. **Melanie Müller** (Universität Siegen, Germany), Peter Betsch (Universität Siegen, Germany) GA/CT2650/004

Assumed enhanced strain (AES) elements (see, for example, [1]) are well-know to exhibit improved convergence behavior, especially in the context of bending dominated situations and in the incompressible limit. In the present work we focus on the application of AES elements to nonlinear elastodynamics. In particular, we aim at the design of energy-momentum schemes for the stable numerical integration of the semi-discrete equations of motion. For this purpose we make use of the notion of a G-equivariant discrete derivative introduced by Gonzalez [2] in the framework of general finite-dimensional Hamiltonian systems with symmetry.

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Energy-momentum schemes for large deformation contact and domain decomposition. **Christian Hesch** (Universität Siegen, Germany), Peter Betsch (Universität Siegen, Germany) GA/CT2649/004

In the present talk large deformation contact problems as well as domain decomposition problems of flexible bodies are addressed within a nonlinear finite element framework.

Actual developments like the mortar method yield a variationally consistent description of the contact surface, see for example, Puso and Laursen [1] and Wohlmuth [2]. This approach passes the patch test and is characterized by a robust behavior.

Over the past years the development of energy and momentum consistent 'mechanical' integrators for the differential algebraic equations (DAEs) have achieved major improvements. Energy consistent mechanical integrators have been recently developed for DAE-formulations of constrained mechanical systems (Gonzalez [3], Betsch and Steinmann [4]).

We aim at the application of the mechanical integrators to the mortar method used for both, contact problems and domain decomposition problems. Special requirements for the algo-

rithmic conservation of energy in the case of high velocity impact are analyzed.

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Two mixed finite-element formulations with area-bubble functions for tetrahedral elements. **Ismail Caylak** (Universität Paderborn, Germany), Rolf Mahnken (Universität Paderborn, Germany) GA/CT1162/004

We address the solution of geometrically linear elastic problems for three dimensional solid mechanics using tetrahedral finite elements. Starting from a five field weak formulation involving fields for conformal displacements, nonconformal displacements, pressure, enhanced strains and stresses, both, the method of incompatible modes and the enhanced strain method are considered as special cases. As a key idea, area bubble functions are used for both mixed finite element formulations in order to enrich the displacement field and the enhanced strain field, respectively. Appropriate conditions for convergence (satisfaction of the patch test) and stability (unique solution of FE-matrix equation) are verified.

In the representative examples firstly a numerical verification of the patch test is obtained. Two additional examples, Cook's membrane problem and a plate with a ring hole, illustrate the good performance of the presented approach in comparison to existing finite element formulations.

Displacement field analysis of the topology optimized structure. **Ryszard Kutylowski** (Wroclaw University of Technology, Poland) GA/CT2990/004

In this paper for the topology optimization process the minimum compliance approach is used with FEM as very useful method for numerical realization of the problem. During the optimization process homogenized domain changes into discrete structure which means the final structure consists of the many optimal placed bars. The analysis of the deformed structure and the deformed elements is done from the displacement field point of view. It can be noticed some of the elements reduce their size, some of them increase their size. It depends on the element status (void-empty, stressed or not stressed).

The question arises: is the topology optimization process cause of the negative Poisson ratio for some parts of the structure?

GA/CTS4533/04: Application of FEM, I.

Organiser: Stefanie Reese (TU Braunschweig, Germany)
Co-organiser: Friedrich Gruttmann (TU Darmstadt, Germany)
Co-organiser: Holm Altenbach (Universität Halle–Wittenberg, Germany)

A locking-free element formulation for 3D nonlinear FE problems. **Markus Kraus** (Universität Erlangen–Nürnberg, Germany), Johannes Geisler (Universität Erlangen–Nürnberg, Germany), Kai Willner (Universität Erlangen–Nürnberg, Germany) GA/CT2559/004

In today's simulations, mechanical systems with large deformations or other nonlinear phenomena are often considered. To solve those problems with the finite element method, isoparametric element formulations with linear shape functions are preferred, due to robustness and computational efficiency. A major disadvantage of these elements is the appearance of locking effects in bending problems and in the limit of incompressibility. These effects occur because of a mere numerical insufficiency of the shape functions that leads to an artifical stiffening of the whole system.

All methods to avoid locking are based on two different techniques. Beside reduced integration with additional stabilization, many formulations are based on mixed variational principles, like the enhanced assumed strain (EAS) method.

In this work a locking free brick element formulation using reduced integration and hourglass stabilization is discussed. In general, the necessary stabilization parameters can be chosen arbitrarily, but here they are derived from an enhanced assumed strain formulation and thus have a real physical character. The element performance is demonstrated in different large deformation problem examples.

Automatic adaptation of the integration formula in thickness direction for solid-shell elements. **Georgios Michaloudis** (Universität Karlsruhe, Germany), Karl Schweizerhof (Universität Karlsruhe, Germany) GA/CT2501/004

In problems with high stretching and intense thickness reduction general three-dimensional material laws as well as strains and stresses in thickness direction are required, imposing the use of *Solid-Shell* formulations. The Solid-Shell elements possess the ability to illustrate directly deformations and stresses in thickness direction, providing the appropriate 3D-continuum discretization, see [1] and [2].

In problems such as metal forming with large deformations where plastic stresses in thickness direction are developed, appears the necessity of a more accurate integration through thickness using more integration points; e.g., Gauss points, increasing respectively the computational time and effort. In this contribution a new algorithm is proposed for the automatic adaptation during the computation of the integration formula in thickness direction. Thus, the computation starts with the minimum required number of integration points in thickness (e.g., two) and during the computation the integration points are increased only in the regions where is needed; e.g., if plastic stresses occur.

Error analysis as well as simple engineering criteria define the time-point and the regions to increase the number of integration points. Application of different integration formulae (e.g., Gauss–Lobatto) in a subdomain integration approach is also presented, see [3] and [4]. The method provides an efficient compromise between accuracy and computational time, as high order integration formulae are applied in an adaptive fashion but only to the elements where and at those time-points when it is needed.

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A novel polygonal finite-element method. **Alexandru Constantiniu** (TU Kaiserslautern, Germany), Paul Steinmann (TU Kaiserslautern, Germany) GA/CT2475/004

In recent years we saw an emerging interest towards using arbitrary polygonal elements in discretization schemes. Latest advances in the construction of interpolants have allowed the use of new building blocks for tessellations, other than n-simplices and regular n-gons.
A novel polygonal finite element method is proposed, based on a hybrid nodal-element approach. Two popular concepts are used, namely Voronoi diagrams and generalized barycentric coordinates. Starting from a classical Delaunay tessellation, we transform it into an adaptive one by subsequently applying a Delaunay circumcenter rule. Polygons are formed by merging simplices intersected by line segments between their barycenters and circumcenters. Constructed in a straightforward and iterative manner, such a tessellation is unique and bounded in computational time. A simple to evaluate form of rational barycentric coordinates for higher dimensions is applied. They have desired properties and reduce to conventional barycentric coordinates in the case of simplices. Over the representative domains around the nodes a stabilized nodal integration scheme is used.
The method has been compared with the classical Delaunay tessellation scheme when applied to scattered data interpolation. A similar interpolation error was obtained, however using approximately 30% fewer elements, with improved geometric properties. Simplices have no angles greater than 90^o, meaning small and large angles are avoided and polygons have as rounded shapes as possible.
Without any predefined connectivity between the nodes, the method can be seen as an extension of the Finite Element Method with which it overlaps for simplices and regular nodal distributions.

Two-grid and hanging-node-based mesh refinement with application to metal forming simulations. **Xin Gu** (Universität Dortmund, Germany), Christian Hortig (Universität Dortmund, Germany), Bob Svendsen (Universität Dortmund, Germany) GA/CT2459/004

In the current work, a two-grid-based h-adaptivity method is combined with a hanging-node based mesh generation approach for application in particular to metal forming simulations. In the h-adaptivity approach, the elements are selected to be refined based on desired mesh density. Hanging node and constraint equation are introduced to handle the transition between different element levels. Alternatively, hanging nodes can be eliminated by using trapezoidal method. In this method, the elements containing hanging node are first split to triangles in an appropriate way, and then the adjacent triangle and quadrilateral which have a common hanging node are merged into a trapezoid. To achieve a prescribed accuracy, a two-grid error estimator controls the h-adaptivity procedure. Example applications of the approach will be discussed.

Aspects of sensitivity analysis using the level-set method in structural optimization. **Monika Rotthaus** (Universität Dortmund, Germany), Franz-Joseph Barthold (Universität Dortmund, Germany) GA/CT1951/004

The level-set method is very common for modelling of structural optimization problems; e.g., multi-material structures. Essentially two different approaches are known. The first method describes the shape by an implicit function. The weak form is expressed as a Heaviside function of this implicit function and the optimization problem is solved by an iterative procedure. This method is applied to topology optimization by e.g., Belytschko et al. [2].

The second approach is based on the combination of the shape derivative and the level-set method for front propagation, which has been devised by Osher and Sethian. Allaire et al. [1] uses the shape derivative for the minimization problem to compute the advection velocity in the Hamilton–Jacobi equation. The Hamilton-Jacobi equation can be solved numerically by an explicit first order upwind scheme on a Cartesian grid.

We propose a new numerical method for shape optimization of multi-material structures. This approach is based on the level-set method combined with the variational sensitivity analysis. The aim of the present contribution is to point out the essential aspects of this combination and to compare it with the two methods mentioned above. Furthermore, the sensitivity of multi-material structures in terms of various design parameters will be discussed.

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Design of cold-formed thin-walled beams with the application of an expert system. **Renata Kasperska** (University of Zielona Gora, Poland), Marian Ostwald (Poznan University of Technology, Poland), Dariusz Mikołajewski (University of Zielona Gora, Poland) GA/CT1797/004

The expert systems are currently used in various disciplines of civil engineering and structural mechanics due to their ability to use symbolic knowledge representations and reasoning capabilities. This paper outlines the application of a knowledge-based expert system built to assist engineers in the designing process and multicriterial optimization of cold-formed thin-walled beams, which are more and more extensively applied in mechanical and civil engineering. The design and implementation of an expert system described in this paper was primarily motivated by a research work on optimal design of thin-walled structures and cold-formed thin-walled beams with monosymmetrical open cross sections conducted by authors and the expert team of Poznan University of Technology, as well as by a study of literature related to the problems of strength and stability of thin-walled beams. In order to develop the expert system, which the overall architecture is presented in the work, a framework called PC-Shell was used. The applied knowledge base includes descriptions of the geometric cross-section characteristics, material and dynamic features of beams and the different discrete and continuous optimization methods, e.g. genetic algorithms. The bi-criteria optimization problem of thin-walled beams is solved on the ground of the minimum in Pareto sense, where beam mass and deflection of the centre of the beam are two optimization criteria. The best optimal solutions are chosen from the set of compromise solutions with the help of preference functions. The work provided optimal parameters of cross-sections of the beams, satisfying the conditions of general and local stability, strength, stiffness of the beam, limiting loading capacity of the beam, structural, technological and exploitation constraints. Results of numerical analysis are presented in the form of tables and diagrams. Plans related to further research are shown at the end of the paper.

GA/CTS4534/04: Application of FEM, II.

Organiser: Bernd Zastrau (TU Dresden, Germany)
Co-organiser: Friedrich Gruttmann (TU Darmstadt, Germany)
Co-organiser: Holm Altenbach (Universität Halle–Wittenberg, Germany)

Least-squares mixed finite elements with applications to anisotropic elasticity and viscoplasticity. **Alexander Schwarz** (Universität Duisburg–Essen, Germany), Jörg Schröder (Universität Duisburg-Essen, Germany) GA/CT2178/004

The objective of this work is to discuss a least-squares finite element method with applications to physically nonlinear and anisotropic constitutive equations at small strains. The L_2-norm minimization of the residuals of the given first order system of differential equations leads to a functional, which is a two field formulation in the displacements and the stresses, see e.g. [1]. In order to approximate the stresses, shape functions related to the edges are chosen. These vector-valued functions belong to a Raviart-Thomas space, which guarantees a compliant discretization of the required space $H(div,\Omega)$. A characteristic attribute of functions $\mathbf{v}$ in $H(div,\Omega)$ is given by its definition $H(div,\Omega) := \{\mathbf{v} \in L^2(\Omega) : div\,\mathbf{v} \in L^2(\Omega)\}$. Furthermore, standard Lagrange polynomials, which are associated with the vertices of the triangle, are used for the continuous approximation of the displacements. A main focus of the presentation lies on the extension of plane elasticity to anisotropic or nonlinear material behavior. In this context we discuss amongst others transversal isotropic elasticity and viscoplasticity. Further on, the governing equations for the considered formulations for the least-squares mixed finite elements are derived and some numerical examples are presented.

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Closest-point projection in contact mechanics: existence and uniqueness for different type of surfaces. **Alexander Konyukhov** (Universität Karlsruhe, Germany), Karl Schweizerhof (Universität Karlsruhe, Germany) GA/CT2454/004

The most important operation for data transfer between contacting bodies in contact mechanics is the closest point projection procedure, where one seeks the projection of a given contact point from one body $\mathbf{r}$, usually called a slave point, onto another contact body, see [1], [2]. The closest point procedure appears also in many other applications such as fluid-structure interactions, computational plasticity etc. The projection problem e.g. for surfaces is usually formulated as an extremal problem

$$\mathbf{F}(\xi^1,\xi^2) = ||\mathbf{r} - \rho(\xi^1,\xi^2)|| \to \min, \quad \longrightarrow (\mathbf{r}-\rho)\cdot(\mathbf{r}-\rho) \to \min, \tag{1}$$

which is solved then mostly numerically. However, then a fundamental problem arises: Does the solution of (1) exist? And, if it exists, then, is it unique for any arbitrary surface approximation? The straightforward answer is given by the result from the convex analysis: if a function $\mathbf{F}(\xi^1,\xi^2)$ is convex in a domain $(\xi^1,\xi^2) \in D$, then the solution of the problem (1) exists and is unique. The goal of the current contribution is to provide this analysis in the local surface coordinate system, introduced for the covariant description of contact problems in [3], [4]. This allows to create a classification of surfaces from its differential geometry point of view onto which a point can be projected uniquely. Thus, a projection domain Ω in 3D can be created a-priori for any arbitrary surfaces including singularities as edges and sharp points, from which any slave point can be uniquely projected onto the given surface. A full set of projection routines is created in order to cover cases with C^2-, C^1- and finally only C^0--continuous situations appearing in practical approximations of arbitrary surfaces.

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A mixed finite-element formulation for piezoelectric shells. **Katrin Schulz** (Universität Karlsruhe (TH), Germany), Sven Klinkel (Universität Karlsruhe (TH), Germany) GA/CT2139/004

A finite element formulation to analyze piezo-electric shell problems is presented. A reference surface of the shell is modelled with a four node element. Each node possesses six mechanical degrees of freedom, three displacements and three rotations, and one electric degree of freedom, which is the difference of the electric potential in thickness direction. The formulation is based on the mixed field variational principle of Hu-Washizu. The independent fields are displacements $\boldsymbol{u}$, electric potential $\boldsymbol{\varphi}$, strains $\boldsymbol{E}$, electric field $\vec{\boldsymbol{E}}$, stresses $\boldsymbol{S}$ and dielectric displacements $\vec{\boldsymbol{D}}$. The mixed formulation allows an interpolation of the strains and the electric field in thickness direction. Accordingly a three-dimensional material law is corporated in the variational formulation. It is remarked that no simplification regarding the constitutive law is assumed. The formulation allows the consideration of arbitrary constitutive relations. The normal zero stress condition and the normal zero dielectric displacement condition are enforced by the independent stress and dielectric displacement fields. They are defined as zero in thickness direction. The present shell element fulfills the important patch tests: the in-plane, bending and shear test. Some numerical examples demonstrate the applicability of the present piezoelectric shell element. *Keywords:* Mixed Field Variational Problem, Finite Element Formulation, Piezoelectricity, Smart Structures, Shells
quad

A variational arbitrary Lagrangian–Eulerian finite-element formulation for standard dissipative solids at finite strains. **Jörn Mosler** (Ruhr-Universität Bochum, Germany), Michael Ortiz (California Institute of Technology, USA) GA/CT1665/004

A novel Arbitrary Lagrangian–Eulerian (ALE) finite element formulation for standard dissipative media at finite strains is presented. In contrast to previously published ALE approaches accounting for dissipative phenomena, the proposed scheme is fully variational. Consequently, no error estimates are necessary and thus, linearity of the problem and the corresponding Hilbert-space are not required. Hence, the resulting Variational Arbitrary Lagrangian-Eulerian (VALE) finite element method can

be applied to highly nonlinear phenomena as well. In case of standard dissipative solids, so-called variational constitutive updates provide a variational principle. Based on these updates, the deformation mapping follows from minimizing an incrementally defined (pseudo) potential, i.e., energy minimization is the overriding criterion that governs every aspect of the system. Therefore, it is natural to allow the variational principle to drive mesh adaption as well. Thus, in the present paper, the discretizations of the deformed as well as the undeformed configuration are optimized jointly by minimizing the respective incremental energy of the considered mechanical system.

Geometrical matrix of Timoshenko beam with nonlinear elastic supports. **Jerzy Rakowski** (Poznan University of Technology, Poland) GA/CT2000/004

The buckling analysis of a beam elastically supported on its ends including the shear-force effect is studied. The general case for the 4-dof beam element supported by springs with arbitrary linear and rotary stiffnesses is considered. The slope-deflection equations for E-B and Timoshenko beams are derived. The closed-form solution of these equations enables one to define stiffness and geometrical matrices for all kinematically and statically possible schemes of beams. The rigid-joint nodes correspond to the infinite-stiffness supports, the free displacement nodes correspond to the zero-stiffness spring supports.The investigations are extended for Timoshenko beams with nonlinear elastic supports. The reactions (forces and moments) are proportional to the third power of support displacements. The adequate slope-deflection equations are derived and the analytical solutions of these equations are given. The influence of support nonlinearity on the Timoshenko beam geometrical matrix and critical forces is analyzed and numerical parameter study is carried out.

The use of an hour-glass stabilized solid-shell finite element in forming simulations: theoretical aspects and first industrial applications. **Marco Schwarze** (TU Braunschweig, Germany), Stefanie Reese (TU Braunschweig, Germany) GA/CT3471/004

To obtain accurate results in finite element simulations of sheet metal forming processes classical three-dimensional solid elements with only displacement degrees-of-freedom have to be modified in the field of finite element technology. The goal is to eliminate the undesired effects of geometrical and material locking and to compute the sheet metal with only one element over the thickness.
One method to avoid locking in non-linear large deformation solid-shell formulations is the method of reduced integration, see e.g. [1-3]. The physically relevant deformation and stress response of the element is computed in a reduced number of Gauss points located on the shell director. To avoid the appearance of non-physical zero-energy modes an hourglass stabilization is necessary. The choice of these stabilization terms is still an object of research, in particular in the case of inelastic material behavior.
We compare the performance of the solid-shell formulation proposed in [1] in combination with different hourglass stabilizations. The goal is to develop an adaptive hourglass stabilization for which no additional user input is necessary. Numerical tests as well as industrial applications are presented.

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04, Posters

GA/PP2166/004: **A coupled MD–FE approach for contact at microscopic length-scales.**

Presenter: Udo Nackenhorst (Leibniz Universität Hannover, Germany)
Co-author: Tobias Helmich (Universität Hannover, Germany)

A model for the electromechanical contact on a microscopic length-scale apparent in an atomic force microscope (AFM) is presented in this contribution. In contrast to classical contact on macroscale, the description on a microscopic length scale has to by physically motivated to ensure realistic simulation results. The contact is modeled by a Molecular Dynamics (MD) approach on a nanoscale with an analytical homogenization in physics. Here a potential formulation of the van der Waals force with a repulsive and attractive component is used for the interaction of two bodies resulting into a continuous contact description where normal– and tangential contributions are coupled consistently. The global system is modeled by a nonlinear Finite Element (FE) approach at the meso–lengthscale. The MD and FE methods are coupled directly by strong coupling via the weak form of the FEM. To encounter the multiscale problem a dimensional adaptive approach is used. Contact, continuum and beam elements, joined by transition elements with different degrees of freedom, are used for the efficient discretization. Numerical examples and results for the introduced coupling strategy are presented for typical AFM setups as fully 3D–simulations.

05, Short Communications

GA/CTS4476/05: **Braking, oscillations.**

Organiser: Roman Bogacz (Institute of Fundamental Technological Research, Poland)
Co-organiser: Roland Pulch (Bergische Universität Wuppertal, Germany)
Co-organiser: Georg Ostermeyer (TU Braunschweig, Germany)

On wear-pattern generation in elastic systems. **Norbert Hoffmann** (TU Hamburg–Harburg, Germany) GA/CT2392/005

Many systems with moving contact show the appearance of regular wear patterns. Examples range from the generation of washboard patterns on dirt roads, to the polygonalization of railway wheels during operation, up to the appearance of thickness variations in the disks of disk brake systems. The origin of the wear patterns is generally thought to be found in the dynamical properties of the contact partners, like e.g. natural frequencies, modal damping, etc. The present work uses some elementary models to elucidate the fundamental mechanisms underlying the wear pattern generation. Two approaches to deal with the coupled structural and wear dynamics are presented. It turns out that wear pattern generation can be understood as an instability phenomenon of the surface evolution, coupled to the dynamical system. The role of structural characteristics, as well as some aspects of the wear model, are discussed. Finally an outlook is given how to extend the present modeling to technically relevant large-scale systems.

Ein Ansatz zur Beschreibung der dreidimensionalen Topographiedynamik bei Bremsvorgängen. **Michael Mueller** (TU Braunschweig, Germany), Georg Ostermeyer (TU Braunschweig, Germany) GA/CT1531/005

Die Dynamik in der Grenzschicht zwischen Bremsbelag und Bremsscheibe ist während eines Bremsvorganges durch eine komplexe Wechselwirkung zwischen Reibung und Verschleiß charakterisiert. Die extrem hohen lokalen Temperaturen, Drücke und die tribochemischen Prozesse führen zum Wachstum und der Zerstörung mesoskopischer, harter und dünner Strukturen auf der Oberfläche des Belages, sogenannter "Patches" [1].

Mit Hilfe eines dynamischen Reibgesetzes [1] und darauf aufbauend einem Modell eines Zellulären Automaten ist es prinzipiell möglich geworden, die Wirkung dieser Prozesse auf makroskopische Reibphänomene anzuwenden [2]. Um weiterhin explizite Aussagen über globale Verschleißraten oder laterale Anregungsmechanismen zu erhalten, ist dieses Modell auf eine dreidimensionale Topographiebe- schreibung erweitert worden.

Zur Verifizierung und Quantifizierung sind identische Bremssysteme mit unterschiedlicher Belastungsgeschichte (von eher gering bis hin zu extrem hoch) optisch untersucht worden. Die daraus gewonnenen Daten der Oberflächentopo- graphie und die Bestimmung charakterisierender Rauhigkeitswerte werden in diesem Paper den Ergebnissen aus der Simulation gegenübergestellt und interpretiert.

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Evaluation of automotive disk brake noise behavior using piezoceramic actuators and sensors. **Stefan Schlagner** (TU Berlin, Germany), Utz von Wagner (TU Berlin, Germany) GA/CT2379/005

Brake squeal is a high-frequency noise of brake systems with frequencies from 1 up to 12 kHz. This noise does not affect the functionality of the brake. Nevertheless it is a serious comfort problem and it causes a high amount of costs to design a noiseless brake system.
The conventional method to evaluate the noise behavior of an automotive disk brake consists usually of realizing different operating conditions several times on a test rig and to measure an existing noise with respect to frequency and intensity by a microphone. This procedure takes a lot of time. The work to be presented shows that with the help of piezoceramic actuators and sensors the noise behaviour of the brake can be examined without making the brake squeal.

Experimentelle Untersuchungen von Stick-Slip-Schwingungen an Scheibenwischern. **Philipp Grönefeld** (Universität Hannover, Germany), Matthias Kröger (Universität Hannover, Germany) GA/CT1548/005

In Kraftfahrzeugen jeglicher Art werden Scheibenwischer zum Reinigen der Windschutzscheibe verwendet. Die Wischerblätter aus Gummi unterliegen dabei hohen Beanspruchungen durch Abgase, Sonneneinstrahlung, Verschmutzungen sowie Eis und Schnee. Die komplexe Reibcharakteristik des Materials führt nach gewissen Parameterzuständen aufgrund einer fallenden Reibkennlinie dazu, dass Stick-Slip-Schwingungen entstehen, die sich durch Rattern und Quietschen des Wischerblattes auf der Scheibe äußern und damit erhebliche Komfort- und Funktionseinbußen nach sich ziehen.

Mit Hilfe unterschiedlicher Prüfstände und Proben werden durch die Variation von Parametern wie Anpresskraft, Geschwindigkeit und Nässezustand verschiedene Belastungen simuliert und die entstehenden Schwingungen untersucht. Die so ermittelten Grenzzykel können Aufschluss über Möglichkeiten zur Optimierung der Wischerkonstruktion geben.

Influence of the non-linear contact stiffness on the vibration behaviour of a tyre tread block. **Matthias Kröger** (Universität Hannover, Germany), Patrick Moldenhauer (Universität Hannover, Germany), Gunnar Gäbel (Universität Hannover, Germany) GA/CT2291/005

In many technical applications, e.g. seals, belts and tyres, the contact of rubber elements influences the dynamical behaviour of the system. In the tyre/road contact friction depends on many parameters like relative velocity, roughness, normal pressure, temperature and material properties. The slip at high rolling speeds causes high-frequency deformations and vibrations.
Within the scope of this work the dynamic behaviour of a tyre tread block is described by a modularly designed model. Special emphasis is laid on the influence of the force-displacement characteristic between rubber and the rough surface. This characteristic is non-linear since at the beginning of the contact process only a small number of surface asperities interacts with the rubber. This leads to a declining contact stiffness characteristic with respect to the normal displacement. In the simulation the rough surface on which the tread block

slides is modelled as smooth with the friction characteristic of the respective material pairing and a non-linear description of the discussed local tyre/road interaction. This leads to an approximate description of the contact mechanics without losing numerical efficiency. Furthermore the model includes wear that changes the block geometry and thus the vibrational behaviour.
With the presented model of a tyre tread block dynamic effects like friction induced vibrations are simulated and compared with experiments conducted on a test rig.

On bending-torsion flutter of a cantilevered beam with tip jet . **J Wauer** (Universität Karlsruhe (TH), Germany) GA/CT1866/005

During the early seventies, several studies on the problem of dynamic instability of cantilevers under transverse follower forces by tip jet and the suppression of the increasing vibrations using feedback control were made. The investigations were based on a simplified geometrically nonlinear theory so that the derived boundary value problem might be imprecise. Some years later, the author presented the academic problem of lateral buckling of such a beam under follower moment tip load of constant magnitude based on a consistent geometrically nonlinear elasticity theory. To possibly improve the modeling of the first problem and to study alternative tip jet concepts, the cantilevered bar under non-conservative transverse fluid loading is re-considered here. In a first step, a consistantly formulated governing nonlinear boundary value is presented. The corresponding variational equations are derived next so that finally, the stability behavior can be analyzed. In addition to damping effects, the ratio of torsional and bending stiffness together with beam slenderness may influence the flutter load in a characteristic manner.

GA/CTS4474/05: Friction, nonlinear oscillations.

Organiser: Alexander Fidlin (LuK GmbH & Co. oHG, Bühl, Germany)
Co-organiser: Roland Pulch (Bergische Universität Wuppertal, Germany)
Co-organiser: Georg Ostermeyer (TU Braunschweig, Germany)

Application of history-dependent friction model to description of excited and self-excited vibration. **Roman Bogacz** (Institute of Fundamental Technological Research, Poland) GA/CT4287/005

In the paper a mechanical frictionally damped system subjected to harmonic excitation and mechanism of generation of stick-slip self-excited vibration is considered. Relatively complicated but piece-wise linear, history dependent friction model is used for description of the friction model. This model was experimentally identified. The friction force in the model depends on: velocity of relative motion, acceleration, sticking time (adhesion), and force rate. Such a friction model enables the description and the analysis of various cases of stationary and transient motion. That is why we can apply it also to the problem of an active control of self-excited mechanical systems. The other advantage of the modeling by the use of piecewise linear friction law is connected with an analytical form of the solution obtained for each linear part of the characteristic. The paper deals mainly with the problem of frictionally-excited vibration of the system, but also reduction or amplification of vibration by means of an additional external excitation of the system with friction will be studied. The system used for verification of the model is composed of an elastically suspended lumped mass made of steel which interacts frictionally with the belt made of composite material. The system additionally can be subjected to a periodic excitation through an elastic element. The simultaneous self-excitation and external periodic force results in occurrence of the solution in the form of one - and higher periodic vibration, quasi - periodic as well as non - periodic (chaotic) oscillation. Results of simulation of some interesting cases will be presented. For example, a case when frictionally self-excited stick-slip vibration are additionally influenced by an external harmonic excitation than for the particular choice of amplitude and frequency of the external excitation it is possible to minimise the amplitude of oscillations more than two times. For majority of parameter values of the external excitation, the amplitude of the system motion is greater then without it. The discussion of appropriate choice of the parameters is given in the paper.

Oscillatory instabilities due to friction. **Hartmut Hetzler** (Universität Karlsruhe (TH), Germany) GA/CT1194/005

Regarding self-excited frictional oscillations, one key issue is to understand the mechanism which triggers the vibrations. Among the most important mechanisms in that context are the so-called "negative damping", leading to divergence instability, and the influence of circulatory forces, which may cause oscillatory instabilies ("flutter"). Over he last decades, the latter effect has been subject of intensive research, revealing the pecularities of circulatory systems. Within this contribution, basic properties of circulatory systems shall be addressed in the context of friction-induced vibrations. Among others, the relation between complex eigenvectors and stability will be discussed as well as the influence of structural damping.

Friction-induced vibrations in a plate/disk. **Gottfried Spelsberg-Korspeter** (TU Darmstadt, Germany) GA/CT2130/005

This paper considers a rotating Kirchhoff plate in contact with two elastic pads. Friction occurs between the disk making the system susceptible for self-excited vibrations. Using the principle of virtual work and the kinematic assumptions from Kirchhoff plate theory the boundary value problem is derived from the basics of the theory of elasticity. Special attention is given to the coupling of disk and plate equations. It is shown that the coupling depends on the interaction between plate and pads and on the assumptions made for the deformation gradient. The insights gained directly from the equations of motion are compared to the results obtained by a Ritz discretization approach. In particular the problem of considering point contact between plate and pads in the continuous approach is addressed.

The results obtained can be used for modelling frictionally self-excited vibrations of disks. They might help to clarify the influence of in-plane modes of the disk on the occurrence of squeal.

The Earth is double system. **Dmitry Kiryan** (Institute of Problems of Mechanical Engineering RAS, Russian Federation) GA/CT3880/001

The Earth's rotation axis moves parallel to itself without changing the angle of inclination to the ecliptic plane. The translational motion of the Earth's axis of rotation is caused by the motion of the Earth's center of mass in the Earth's body. The motion of the Earth's center of mass in space is due to the motion of the consistent inner core of the Earth in the liquid outer core under the action of the total (internal and external) gravitational field. The comparison of our calculations and observational data on variations in "latitudes" of places and acceleration of gravity has shown that they are in good agreement. Our model has been shown to adequately describe the physical process of motion of the Earth's centre of mass inside the Earth's body.

Analysis of the vibration behavior of the Dobson space telescope. **Kerstin Kracht** (TU Berlin, Germany), Utz von Wagner (TU Berlin, Germany), Ulrik Strehlau (TU Berlin, Germany) GA/CT2357/005

The Dobson Space Telescope is a research project of TU Berlin. Aim of the project is to develop a new type deployable space telescope that can overcome the mass and volume limitations of cost effective micro satellites. Due to the deployable structure of the telescope there are two basic questions referring to mechanical vibrations. Firstly, what is the behaviour of the folded structure during launch? Secondly, do the vibrations of the deployed telescope allow the production of high quality photos?

The author has analyzed the vibration behavior of the Dobson Space Telescope. This paper gives an overview about the results of the metrological modal analysis and of analytical and numerical calculations. All results show that the aluminium lab model of the telescope would be ready for service referring to the aspect of mechanical vibrations.

Coupled nonlinear oscillations in compressed thin-walled bars. **Arkadiy Manevich** (Dnipropetrovs'k National University, Ukraine) GA/CT2615/005

In thin-walled bars the spectrum of short-wave local modes is usually rather dense, and natural frequencies for overall and some local modes can be commensurable: their ratio can be close to 1:1, 2:1 and so on. Under action of axial force the external parametrical resonance may take place simultaneously with internal resonances of various types, such as one-to-one resonance, auto-parametrical or combination resonance. In the paper the nonlinear oscillations in thin-walled bars caused by the compressive and harmonic axial forces are studied with taking into account the interaction of overall and local modes. It is assumed that the bar has one axis of symmetry, and the natural frequencies for the overall mode and certain local mode are close. Equations of motion are derived based on assumption that the natural modes of oscillations coincide with the buckling modes (it is the case, in particular, for simply supported bars). The dynamic displacements field is expanded in a series in natural buckling modes (the KoiterŠs type expansion for the static buckling problem). The equations of motion in the first nonlinear approximation comprise quadratic nonlinearities due to interaction of the modes. These equations have been solved by the multiple scale method. Equations of amplitudeŰfrequency modulation have been obtained and analysed. It is shown that the interaction of the external parametric and internal resonances gives rise to complex nonlinear phenomena. The energy exchange between different modes can lead to appearance of new steadyŰstate coupled oscillations and coupled non-stationary oscillations. Such a complicated behavior can cause loss of stability in certain mode because of accumulation of energy on this mode.

GA/CTS4477/05: Rotations, stability.

Organiser: Norbert Hoffmann (TU Hamburg-Harburg, Germany)
Co-organiser: Roland Pulch (Bergische Universität Wuppertal, Germany)
Co-organiser: Georg Ostermeyer (TU Braunschweig, Germany)

Analysis of the stator/rotor-contact in a two-stators hybrid-transducer-type ultrasonic motor. **Nantawatana Weerayuth** (Universität Karlsruhe, Germany), Wolfgang Seemann (Universität Karlsruhe, Germany) GA/CT2260/005

In this paper, a new procedure to understand the contact mechanism of an ultrasonic motor by using finite-element analysis is presented. First, the modes of vibration of a stator will be calculated and be analysed using a commercial finite element program package ANSYS. The distribution of elliptic path of motion of nodes on the stator surface is studied. The computed resonance frequencies of the stator are compared with the measured one by using the precision impedance analyzer AGILENT 4294A. Finally, the contact conditions, normal displacement, normal velocity, tangential velocity and friction force between stator and rotor will be calculated.

Modellierung der Schwingungen beim Werkzeugschleifen. **Lars Panning** (Leibniz Universität Hannover, Germany), Matthias Kröger (Universität Hannover, Germany) GA/CT1984/005

Die Fertigung von Bohrern und Schaftfräsern aus Hartmetall oder Schnellarbeitsstahl (HSS) erfolgt aufgrund der großen Härte der Werkstücke häufig durch Profilschleifprozesse mit Diamant- oder CBN-Schleifscheiben. Aufgrund der Wechselwirkung zwischen Werkstück, Schleifscheibe und Prozess kommt es während der Erzeugung der Spannuten zu Werkstückschwingungen, die zu unerwünschten Fertigungsungenauigkeiten und Formfehlern führen. Ziel ist es, mit Hilfe von Simulationen kritische Prozessparameter zu ermitteln, bei denen z.B. durch regeneratives Rattern instabile Zustände auftreten. Diese können die Werkstückqualität erheblich reduzieren.

Es wird ein Simulationsmodell vorgestellt, das den beim Werkzeugschleifen hohen Materialabtrag und die statischen und dynamischen Nachgiebigkeiten des weit auskragenden, schlanken Werkstücks berücksichtigt. Insbesondere wird die sich während des Prozesses stark ändernde Masse und Steifigkeit des Werkstücks betrachtet und in ein mechanisches Ersatzmodell umgesetzt. Die Kopplung zwischen Schleifscheibe und Werkstück erfolgt über ein Prozessmodell, das diskrete, in der ausgedehnten räumlichen Kontaktzone auftretende Prozesskräfte berücksichtigt. Hierzu wird die Eingriffsgeometrie in jedem Zeitschritt unter dem Einfluss dynamischer Relativverlagerungen ermittelt und das Zerspanvolumen in radialer, axialer und in Umfangsrichtung diskretisiert. Anschließend werden die Prozesskräfte in Abhängigkeit der diskreten Volumina ermittelt. Unter Berücksichtigung der momentanen dynamischen Eigenschaften des Werkstücks können nach erfolgter Kopplung des Struktur- und Prozessmodells kritische Bearbeitungszustände detektiert werden, deren Vorhersage und Vermeidung für die Erzeugung qualitativ hochwertiger Werkstücke unerlässlich ist.

Modeling of jointed structures using zero thickness interface elements. **Johannes Geisler** (Universität Erlangen-Nürnberg, Germany), Kai Willner (Universität Erlangen-Nürnberg, Germany) GA/CT2185/004

An important contribution to global damping of mechanical devices is *structural damping* in joint interfaces. The mechanism of structural damping is energy dissipation due to frictional effects in contact areas of joints. In order to investigate the mechanical behaviour in joint interfaces numerically, a contact element in the context of the Finite Element Method (FEM) is presented. The suggested element is an isoparametric zero thickness element which is well suited for the present problem because the contact area is known and only small relative displacements occur.

In these elements arbitrary linear or nonlinear constitutive contact models for normal and tangential contact behaviour can be implemented. Using a proper parametrisation of the contact

area, it is possible to apply the element in contact interfaces lying arbitrarily in space and in interfaces discretized with distorted elements.

In joint interfaces it is undesirable that gross slip occurs, i.e. only mircroslip effects take place. So the constitutive element formulation has to be able to model these effects properly. Different numerical examples are shown and compared with experimental results.

Modelling of rotating shafts with flexible disks. **Jakub Šašek** (University of West Bohemia, Czech Republic), Vladimír Zeman (University of West Bohemia, Czech Republic), Michal Hajžman (University of West Bohemia, Czech Republic) GA/CT1922/005

The dynamic analysis of high-speed drives and their operation conditions call to more complex mathematical models, for which it is needed to develop new modelling approaches. The vibration analysis of driving mechanisms is commonly performed with the assumption of ideal rigid disks mounted on flexible shafts. However, there are cases in which the vibration of disks become important and the rigid body assumption is too rough for detailed dynamic analysis. This assumption is not correct in the case of the high frequency excitation and therefore it is necessary to care about special approaches to the modelling of rotating shafts with flexible disks. There are no difficulty in modelling rotors using standard commercial FEM tools, but such codes usually do not take into account the all effects caused by the rotation.

This paper deals with the methodology of the modelling of rotating shafts with flexible disks. Rotating shafts are modelled as a one dimensional continuum on the basis of the Bernouli-Euler theory, which assumes that the shaft cross section remains a flat plane and is perpendicular to the centerline during vibration. Disks are modelled as a three dimensional continuum by means of the finite element method. The presented approach allows to introduce centrifugal and gyroscopic effects. The special coupling matrix is used for connecting the rotating shaft and mounted flexible disk.

Because vibration analysis of gear-shaft-bearing systems is a very important part of rotor dynamics, the gear connection matrix between two flexible wheels mounted on the particular shafts is also developed and presented in the paper. The whole flexible geared-disk-shaft-bearing system is fixed to the rigid frame by the rolling element bearings. The proposed modelling methodology is used in the example of the simple system composed of two coupled shafts with gears.

On conditions of flutter onset for elongated plate in supersonic gas flow. **Boris Loginov** (Ulyanovsk State University, Russian Federation), Oleg Makeev (Ulyanovsk State University, Russian Federation) GA/CT1787/005

The considered problem is described by the nonlinear equation [1]

$$\frac{\gamma}{g}\frac{\partial^2 w}{\partial t}+\varepsilon\frac{\partial w}{\partial t}+\frac{D}{h}\frac{\mathrm{d}^2}{\mathrm{d}x^2}\left(\frac{w''}{(1+w'^2)^{3/2}}\right)=\frac{1}{h}p_0\mathcal{K}(w',M,\gamma)+\frac{Eh}{a(1-\nu^2)}w''\int_0^a[(1+w'^2)^{1/2}-1]\mathrm{d}x \qquad (1)$$

for two types of boundary conditions I. $w(0,t)=0$, $w''_{xx}(0,t)=0$, $w(a,t)=0$, $w''_{xx}(a,t)=0$ (hingely fastened edges); II. $w(0,t)=0$, $w'_x(0,t)=0$, $w(a,t)=0$, $w'_x(a,t)=0$ (both edges are rigidly fixed), where w is the deflection of the plate, h – its thickness, a – its width, $D=\frac{Eh^2}{12(1-\nu^2)}$ the stiffness, E the Young module, ν is the Poisson coefficient, ε the linear damping coefficient, γ is the density of the plate; M is the Mach number, p_0 – the pressure and γ – the polytropic exponent, g – the acceleration of gravity; $\mathcal{K}(w',M,\gamma)$ is nonlinear differential operator describing the aerodynamic action.

According to Lyapounov-Schmidt method for dynamic bifurcation [2] the linearized equation (1) in dimensionless variables is reduced to the problem $u^{(4)}(x)+\sigma u^{(1)}(x)-\alpha^2\frac{A}{\chi^2}=0$ for complex-valued function $u(x)$ with boundary conditions of the type I and II ($a=1$, σ is proportional to M). It is shown that the boundary condition determinants have simple roots and the rank of the relevant matrices is equal to 3. Consequently the existence of oscillatory solutions for the problem (1) is equivalent to the existence of simple pure imaginary eigenvalues $\pm i\alpha$.

1. Vol'mir A.S. Stability of deformated systems. Moscow, GIFML. 1964

2. Loginov B.V. Determination of the branching equation by its group symmetry – Andronov-Hopf bifurcation. Nonlinear Analysis TMA 28, no. 12, 2033–2047 (1997).

Dynamic stability of disks subjected to rotating in-plane edge loads. **Tyau-Her Young** (National Taiwan University) GA/CT4036/005

The vibration and stability behavior of a spinning disk under a space-fixed in-plane edge load have attracted researchersŠ attention because of its potential application in such fields as spur gear transmission, grind wheel operation and circular saw cutting. But the presence of the initial stress and the Coriolis force that arise due to the rotation of the disk and the presence of the initial stress due to the in-plane edge load which has relative motion with respect to the disk make the problem quite complicated. Therefore, this problem is sometimes simplified by either neglecting the rotation effect of the disk or neglecting the relative motion between the load and the disk.

This paper studies the dynamic stability of a stationary annular plate subjected to a static in-plane edge force moving around the circumference of the disk with a constant speed. Due to this rotating in-plane edge load, the stress field is a periodic function of time, and parametric excitation is observed in the equation of motion when the analysis is conducted in an inertial coordinate system. First the rotating in-plane edge load is expanded into a Fourier series. Next a stress analysis is carried out to determine the initial stress distributions caused by the rotating edge load. Then the finite element method is applied to yield the discretized equations of motion. Finally, the method of multiple scales is adopted to derive the stability boundaries of the disk.

Numerical results show that if the rotating in-plane edge load has a tangential component, there exists a critical damping factor below which the disk is unstable no matter what rotating speed the in-plane edge load is. For disks with a damping heavier than the critical damping factor, combination resonance of the summed type , where is the rotating speed of the in-plane edge load, and are the pth and qth natural frequencies of the disk, may exist, but not combination resonance of the difference type.

GA/CTS4435/05: Oscillations, bifurcations.

Organiser: Georg Ostermeyer (TU Braunschweig, Germany)
Co-organiser: Roland Pulch (Bergische Universität Wuppertal, Germany)

Stability analysis of non-conservative mechanical systems via optimization. **Nils Wagner** (Universität Stuttgart, Germany) GA/CT979/005

The generalized eigenvalue problem $K x = \lambda M x$, where K and M are $n \times n$ real matrices with M being symmetric positive definite, arises in many applications, most notably in structural dynamics. A major difficulty is the stability analysis of such systems, when the matrices are parameter dependent. Since the stiffness matrix K is nonsymmetric the pencil (K, M) is known to admit complex eigenvalues.

Nowadays, these matrices are large, sparse and only a few of the eigenvalues and the associated eigenvectors are desired.

Following Auchmuty several objective functions are used to solve the eigenproblem via (unconstrained) optimization. Finally, a numerical algorithm is proposed for computing an arbitrary eigenpair of the matrix pencil. Knowledge of (K, M) is only required through a routine that performs matrix-vector products.

Hopf bifurcations of travelling waves in a brake-like system. **Alois Steindl** (TU Wien, Austria) GA/CT1874/005

We consider a system composed of an elastic tube, which is fixed at the outer boundary and in frictional contact with a rigid cylinder, rotating inside the tube about the common axis. Under the assumption of Coulomb's friction law at the contact surface between the two bodies several types of rotating slip-stick and also slip-stick-separation travelling waves with different wave numbers can be observed.

For a wide range of parameters the linearized system has unstable complex eigenvalues, which cause high frequency oscillations and unpleasant squeal. We try to locate the stability boundaries in parameter space and determine the oscillatory motion in the unstable regime.

Analysis of the effect of bending stiffness on slender continua in stationary motion. **Ulrike Zwiers** (Universität Duisburg-Essen, Germany) GA/CT2103/005

Studies concerned with the dynamics of belt-drive systems are commonly based on either second-order string models or fourth-order beam models. While the former exhibit non-dispersive wave propagation, the latter possess both propagating and non-propagating waves due to the dispersive nature of flexurally stiff continua.

This talk addresses the transition from perfect flexibility to flexural rigidity. First, the problem of stationary motion is defined, and it is demonstrated that a perfectly flexible string can undergo a snake-like motion, that is, a motion along an arbitrary fixed path in space only at constant speed. Furthermore, the geometric shape of a flexurally stiff continuum in stationary motion is shown to coincide with the static shape. For the special case of motion along a straight line, the linear equations of motion governing the transverse vibrations of a flexurally stiff continuum in axial motion are obtained by superposing small perturbations on the stationary solution. Referring to a belt drive as a typical application of the problem, the definition of appropriate boundary conditions is briefly discussed and the closed-form solutions of the corresponding boundary-value problems are presented. The natural frequencies are determined by applying the phase-closure principle which provides further insight into the wave propagation in axially moving continua.

On the nontrivial interaction of strongly-damped mechanical systems with high-frequency excitation. **Alexander Fidlin** (LuK GmbH & Co. oHG, Bühl, Germany) GA/CT2234/005

Nontrivial effects of high-frequency excitation on mechanical systems have been investigated intensively in the last decade. However, the main attention is normally paid to weakly damped systems which are usual in mechanical applications. In that case the strong high-frequency excitation terms are balanced with large inertial forces (i.e. acceleration terms which are proportional to the frequency square). There are at least two research and applications areas where the situation is significantly different. It is quite usual to apply strong damping to control systems. The reason for that is the objective to avoid unnecessary oscillations and to lead the controlled system for example to its final position as soon as possible. Fast vibrations are often used in control systems either in form of vibrational control or in order to smoothen the effective dry friction. The interaction of this fast excitation (if it is sufficiently strong) with strong damping terms can cause undesired phenomena irritating the control system. Another and perhaps even more important area are micro systems. It is almost obvious that inertial terms are proportional to the mass of the system, i.e. to the cube of its linear dimension. The damping forces are usually applied to the surface of the body. Thus they have to be proportional to the square of the linear dimension. Decreasing linear dimension increases the importance of the damping terms. This paper investigates nontrivial effects occurring if a strongly damped mechanical system is subjected to strong high-frequency excitation. The analysis is focused on the differences between the classic results well known for weakly damped systems and new effects for which the large damping terms are responsible.

Codimension-1 bifurcations of a friction oscillator. **Andreas Teufel** (TU Wien, Austria), Hans Troger (TU Wien, Austria), Alois Steindl (TU Wien, Austria) GA/CT2333/005

In [1] the complete list of all codimension-1 (1-parameter) bifurcations for discontinuous planar piecewise smooth autonomous systems, which are called Filippov systems, is given. By means of the standard model of the friction oscillator, where a mass which is elastically supported is in frictional contact with a rough moving belt, we study for increasing the speed of the moving belt the sequence of qualitative changes in the phase plane. This will be done in a systematical way by comparison with the classification in [1] for different parameter combinations in a three parameter law of the friction force depending on the relative velocity.

Further we show for a more complicated (infinite dimensional) friction system, i.e., a rigid shaft rotating with frictional contact in a space fixed elastic tube that due to the more complicated mechanical model already for simpler friction laws similar effects are possible as for the simpler mechanical model with more complicated friction law.

[1] Kuznetsov, Yu.A., Rinaldi, S. and Gragnani, A.; One-Parameter Bifurcations in Planar Filippov Systems. International Journal of Bifurcation and Chaos, Vol. 13, No. 8 (2003) pp.2157–2188.

Gyroscopic stabilization and destabilization in non-conservative systems. **Oleg Kirillov** (Lomonosov Moscow State University, Russian Federation) GA/CT496/005

Stability of a linear autonomous non-conservative system in presence of potential, gyroscopic, dissipative, and non-conservative positional forces is studied. The cases when the non-conservative system is close to a gyroscopic system or to a circulatory one, are examined. It is known that the marginal stability of gyroscopic and circulatory systems can be destroyed or improved up to asymptotic stability due to action of small non-conservative positional and velocity-dependent

forces. The present contribution shows that in both cases the boundary of the asymptotic stability domain of the perturbed system possesses singularities such as "Dihedral angle" and "Whitney umbrella" that govern stabilization and destabilization. Approximations of the stability boundary near the singularities and estimates of the critical gyroscopic and circulatory parameters are found in analytic form. In case of two degrees of freedom these estimates are obtained in terms of the invariants of matrices of the system. As an example, the asymptotic stability domain of the modified Maxwell-Bloch equations is investigated with an application to the stability problems of gyroscopic systems with stationary and rotating damping, such as the Crandall gyropendulum, tippe top and Jellet's egg.

GA/CTS4475/05: Oscillations, vibrations.

Organiser: Roland Pulch (Bergische Universität Wuppertal, Germany)
Co-organiser: Georg Ostermeyer (TU Braunschweig, Germany)

On the extension of Brommundt's solution to the Painlevé paradox. **Florian Fischer** (TU Darmstadt, Germany) GA/CT2774/005

Painlevé's paradox for dry friction was formulated in 1895 and deals with the contradiction appearing in a rigid, inhomogeneous cylinder rolling on a rigid and rough surface. An analysis based exclusively on rigid body dynamics results in singularities and abnormal values for the contact forces. Recently (2003) Brommundt has shown that introducing elasticity in the normal direction and adding an additional degree of freedom leads to the resolution of the paradox and to vibrations of high frequency in the normal direction. This note extends Brommundt's approach to multiple, discrete and elastic bodies interacting by a stiff coupling. From the equations of motion it can be seen that self-excited vibrations occur. The results can be used to resolve inconsistencies arising in multi-body codes.

On the dynamics of a nonlinear rotor-floating ring bearing system. **Aydin Boyaci** (Universität Karlsruhe (TH), Germany), Carsten Proppe (Universität Karlsruhe, Germany), Wolfgang Seemann (Universität Karlsruhe, Germany) GA/CT2353/005

Today, in high speed applications the rotors are commonly supported by hydrodynamic journal bearings. One typical configuration of journal bearings incorporated in automotive turbochargers is the floating ring bearing. Rotors supported by floating ring bearings have many advantages for example with regard to costs and power consumption. However, they might become unstable with increasing speed of rotation. At the onset of instability both the perfectly balanced and unbalanced rotor undergoes self-excited vibrations which could cause the mechanical breakdown of the system. This phenomenon of *oil whip* is very well known from the investigations of the plain journal bearing occurs here in a different form. At the stability limit the rotor begins either oscillating with about the half of the ring speed or the half of the ring speed plus the half of the journal speed depending on the system parameters.

For this reason a rotor-floating ring bearing model is presented showing the mentioned characteristics. By applying the nonlinear equations of motion the limit cycles of the system are determined and its loss of stability is investigated. Furthermore, the influence of the rotor-bearing design parameters on the stability of the system is discussed.

Influence of internal parametric and kinematic gearing excitation on nonlinear gearbox vibration. **Miroslav Byrtus** (University of West Bohemia, Czech Republic), Vladimír Zeman (University of West Bohemia, Czech Republic) GA/CT1892/005

The mathematical modelling of nonlinear gearbox vibration is based on the system decomposition into linear subsystems (shafts with gears and a housing) and on discretization of nonlinear couplings between subsystems. The final condensed mathematical model is created by means of spectral and modal submatrices corresponding to the lower vibration mode shapes of the mutually uncoupled and undamped subsystems.

The rotating shafts are joined mutually by gear couplings and are linked up by rolling-elements bearings with the housing. The bearing model respects real number of rolling bodies and real roller nonlinear contact forces acting between journals and the outer housing in dependance on their deflection. The nonlinear gearing model enables to consider such vibration, when in consequence of low static load and internal excitation generated in gear meshing, the gear motion is characterized by the gear mesh interruption. Therefore vibrations are accompanied by impact motions, bifurcation of solution and chaotic motions. We consider two main excitation sources, the internal kinematic excitation in gearing caused by kinematic transmission errors and the parametric excitation caused by periodic change of m and $m+1$ teeth in gear meshing. Because of this change the meshing stiffness is described by a time varying function, whose accurate evaluation can be performed by using the theories proposed by many authors.

The influence of simultaneous internal kinematic and parametric excitation is investigated for different levels of external static loading of the gearbox in dependance on revolutions of the driving shaft.

The gear drive motions are explained by applying time-integration method to the condensed model by means of phase trajectories of gearing and bearing deformations. The presented approach to the nonlinear vibration analysis of the large multibody gear drives is illustrated on a real car gearbox.

Dynamics of space systems with pendular elements. **Alexander Burov** (Russian Academy of Sciences, Moscow) GA/CT2252/005

Dynamics of Orbital Systems with pendular elements is a subject of intensive investigations, in particular, within the frame of the programme of creation of Orbital Tethered Systems and Terrestrial and Lunar Space Elevators. In the talk one discusses the problems of existence and stability of steady configurations of Space Pendula within the various assumptions, as well as regular and chaotic dynamics of Space Pendula subjected to periodic excitations.

Model of the axial load of the band-saw. **Jozef Wojnarowski** (Silesian University of Technology, Gliwice, Poland) GA/CT3704/005

The paper presents a model of load exerted on the self-aligning head of a cutting machine. The formulated model concerns the proper conditions of exploitation of the cutting machine, preventing of slips of the saw on the wheels. The endless band-saw is spread between two wheels, after which the tension recommended by the producer is applied. The tension is expressed in units of the mean tension in the saw: for metal-cutting saws it has been assumed within the range of 200-250 MPa. Depending on the type of the cutting machine, the band-saw is twisted in the cutting zone by means of two guides 4, 8 at a constant angle, generally not exceeding 900 (Fig.1). The guides facilitate the attainment of the pre-set geometrical properties of the surface at the kerf. The maximum value of the axial load exerted on the saw occurs at its contact with the driving wheel. The diagram is based on the assumption that the applied values of the forces do not change with time. Ac-

tually, this does not fully comply with reality. The first reason for this are the vibrations in the driving system. The second reason, implicating the former one, is the continuous getting in mesh and out of mesh of the subsequent teeth in the cutting zone. In order to investigate the character and progress of changes of the impulsive cutting force a device with dynamic force sensors has been designed and constructed, installed in vice. This device, , permits to measure the impulsive load Pz transmitted to the device in cutting zone of the saw teeth The analysis of the obtained results has shown that the spectrum of the measured force contains a component which is specific for the applied pitch of the saw and its speed, which value depends on the loading of the teeth and can be used for the automatic control of the instantaneous value of the pressure force of the saw exerted on the object 6that is being cut, depending on the changing conditions of cutting. Experimental investigations have shown that the application of the measurement system (which measures cutting force) allows to adjust the pressure force of the bandsaw on a workpiece. The adjustment strategy takes into account the current cutting parameters, e.g. by detecting the characteristic components of the spectrum of force.

GA/CTS4478/05: Oscillations, miscellaneous.

Organiser: Alois Steindl (TU Wien, Austria)
Co-organiser: Roland Pulch (Bergische Universität Wuppertal, Germany)
Co-organiser: Georg Ostermeyer (TU Braunschweig, Germany)

Investigations on the wire-slicing process. **Thomas Liedke** (TU Bergakademie Freiberg, Germany), Alfons Ams (TU Bergakademie Freiberg, Germany) GA/CT3778/005

The wire slicing technology plays an important role on the manufacturing of thin discs out of brittle materials and is used for example in the solar- and microchip industry. The surface of a wire sliced disc shows a characteristic geometry, which suggest the influence of oscillations in the slicing process. In order to examine the process a distinct-element-model is used to simulate the motion and the interaction of the slicing-particles with the moving wire and the workpiece. The simulation shows interesting phenomena like clustering of particles and reacting forces to the wire, which could be one reason for the observed oscillation in the process.

Partial differential–algebraic equations for simulating frequency-modulated signals. **Roland Pulch** (Bergische Universität Wuppertal, Germany) GA/CT4251/005

In radio frequency applications, signals with widely-separated time scales arise in electric circuits. For example, the amplitude and/or frequency of fast oscillations is changed by slowly varying signals. A multidimensional modelling of these signals allows for an alternative approach in a numerical simulation, since the time scales are decoupled. The representation of frequency modulated signals leads to warped multirate partial differential algebraic equations. Initial-boundary value problems or biperiodic boundary value problems have to be solved according to the underlying periodicities in the signals. Moreover, the adequate determination of an arising local frequency function is crucial for the efficiency of the model. We present strategies based on minimisation criteria to identify a suitable local frequency function. Numerical simulations using the resulting conditions are performed.

Stochastic oscillations in circuit simulation. **Thorsten Sickenberger** (Humboldt-Universität zu Berlin, Germany), Renate Winkler (Humboldt-Universität zu Berlin, Germany) GA/CT4111/005

Due to parasitic effects in integrated circuits it becomes desirable to take noisy elements into account. As a consequence the underlying circuit equations are extended by an additional stochastic part, which extends the differential-algebraic equation (DAE) to a stochastic differential-algebraic equation (SDAE).
We present an adaptive simulation method for an ensemble of solution paths, which is computed simultaneously. The control strategy is based on estimating the time-discretization and the sampling error during the numerical integration. This approach provides a framework for efficient transient noise analysis of oscillatory circuits as well as of non-oscillatory circuits.

Finally we will illustrate the results of the simulation of some real-life problems and show their different behaviour in a noisy environment.

On the influence of crosswind on the overturning stability of railway vehicles. **Christian Wetzel** (Universität Karlsruhe, Germany), Carsten Proppe (Universität Karlsruhe, Germany), Claire Yalamas (Universität Karlsruhe, Germany) GA/CT1189/005

In recent years modern railway vehicle design shows a trend to faster, lighter and more energy efficient railway systems. These developments unfortunately alter the crosswind stability in a negative manner and so the risk of overturning of railway vehicles during operation in strong winds becomes a critical issue. The risk of overturning is quantified by the probability that a railway vehicle capsizes. To improve the crosswind stability it is very important to know the influence of the design and excitation variables on the wheel unloading of the railway car. The wheel unloadings of the windward wheels are the most critical factors. Sensitivities of the design and excitation variables with respect to the probability of failure are calculated and the most influential variables are accentuated. To get a deeper insight of the behavior of the railway system it is essential to model the railway vehicle and the environment as realistic as possible. This means that especially the wind excitation has to be modeled very precisely taking the turbulent fluctuations and track irregularities into account. In this talk results of the mentioned investigations are shown.

A proof of Mikota's conjecture. **Wolfgang Weber** (TU Dresden, Germany) GA/CT5053/005

In 2001 Mikota designed a chain structured mass–spring vibration system with n degrees of freedom. Mikota developed special distributions for spring stiffnesses k_i and masses m_i, each coupled to n and the coordinate x_i. Furthermore the k_i are depending on a basis-stiffness k as the masses m_i depend on a basis-mass m. According to Mikota this arrangement leads to natural frequencies $\Omega_i = i\Omega$ whereas $i = 1, \ldots, n$ and $\Omega = \sqrt{k/m}$. The presentation will prove the aforementioned supposition.

06, Short Communications

GA/CTS4479/06: **Inelasticity of polymers and elastomers.**

Organiser: Herbert Baaser (Freudenberg AG, Germany)
Co-organiser: Alexander Lion (Universität der Bundeswehr, Germany)
Co-organiser: Rolf Mahnken (Universität Paderborn, Germany)

Finite thermo-viscoplasticity of amorphous glassy polymers: experiments, modeling and simulations. **Serdar Göktepe** (Universität Stuttgart, Germany), Joel Méndez (Universität Stuttgart, Germany), Christian Miehe (Universität Stuttgart, Germany) GA/CT4005/006

The contribution is concerned with experimental procedures, constitutive modeling and the algorithmic implementation of thermomechanical coupling effects in rate-dependent finite plasticity of glassy polymers. The experimental investigations involve both homogeneous and inhomogeneous tests at varying temperature levels. The true stress-strain curves obtained from homogeneous uniaxial and plane strain compression experiments are employed for the identification of the adjustable parameters in the proposed three dimensional constitutive model. In addition to load-displacement curves obtained from inhomogeneous experiments, non-uniform distributions of deformation fields are presented, such as thickness changes along a dumbbell-shaped specimen. The facility employed for the optical measurement of the deformation fields is equipped with CCD cameras and a post-processing software. In contrast to the existing kinematic approaches to finite plasticity of glassy polymers, we propose a distinct kinematic framework constructed in the logarithmic strain space. The logarithmic framework is extremely attractive due to the fact that it allows a very efficient algorithmic treatment of the finite plasticity akin to geometrically linear theory. The evolution law of plastic strains is adopted from Arrhenius-type rate formulations that are based on the one-dimensional micromechanically motivated approaches. The proposed formulation is algorithmically implemented and used for finite element analyses of three-dimensional boundary value problems. The model parameters determined from homogeneous experiments are further validated by simulating the inhomogeneous experimental data involving the optical field measurements.

Vergleichende Messungen und Simulationen annähernd homogener Belastungsverteilungen. **Carsten Hohl** (Universität Hannover, Germany), Thomas Alshuth (Deutsches Institut für Kautschuktechnologie, Germany), Jörn Ihlemann (Deutsches Institut für Kautschuktechnologie, Germany) GA/CT3682/006

Zur Charakterisierung und Prüfung technischer Gummiwerkstoffe werden häufig Messmethoden herangezogen, deren Ziel die Erfassung einer möglichst homogenen Verteilung von Spannungen und Verzerrungen ist. Die am besten bekannte und bei weitem am häufigsten durchgeführte Messmethode dieser Art ist die Zugbelastung von S2-Probekörpern. Diese Probekörper weisen zwischen den beiden für die Einspannung vorgesehenen Enden einen schlanken prismatischen Mittelteil auf, in dem sich bei der Belastung eine weitgehend homogene einachsige Belastung einstellt. Diese Belastung wird durch die aufgebrachte Gesamtkraft und die unmittelbar am Mittelteil gemessene Längung erfaßt. Weitere Beispiele für Standardmessmethoden sind kombinierte Zug- / Druckversuche an rotationssymmetrischen Hantelprüfkörpern, Druckversuche an zylindrischen Prüfkörpern sowie mehrachsige Zug- und einfache Scherbelastungen.

In einigen dieser Fälle werden mit unterschiedlichen Messmethoden die gleichen Belastungsarten erzeugt. Darüber hinaus ergeben sich aus der annähernd vollständigen Inkompressibilität der Gummiwerkstoffe weitere Vergleichsmöglichkeiten. Beispielsweise sollten im Idealfall bei einer äquibiaxialen Zugbelastung und beim einachsigen Druckversuch identische Verzerrungszustände erzielt werden. Die gemessenen Spannungen sollten sich dementsprechend durch eine Umrechnung des hydrostatischen Drucks ineinander umrechnen lassen.

Abweichungen von den prinzipiell zu erwartenden Übereinstimmungen erklären sich zum Teil aus Unterschieden in den Materialeigenschaften, die aus der Vulkanisation unterschiedlicher Geometrien herrühren können. Neben eigentlichen Messfehlern kommen Abweichungen von der homogenen Spannungs- / Verzerrungsverteilung in den vermessenen Materialbereichen als weitere Erklärungen für Abweichungen von den theoretischen Erwartungen in Frage. Der Grad der in den verschiedenen Messmethoden erreichten Homogenität läßt sich durch FEM-Simulationen der realisierten Belastungen unter Einsatz geeigneter Stoffgesetze erfassen. Gleichzeitig stellt ein breites Testprogramm unterschiedlicher Belastungsarten am gleichen Material eine weitreichende Möglichkeit zur Beurteilung der Anpassbarkeit und damit der Praxistauglichkeit der verwendeten Stoffgesetze dar.

Experimental and numerical investigations of a compressible cellular rubber. **Michael Johlitz** (Universität des Saarlandes, Germany), Holger Steeb (Universität des Saarlandes, Germany), Stefan Diebels (Universität des Saarlandes, Germany) GA/CT3625/006

Cellular rubbers are multifarious used in the automobile industry; e.g. in the construction of gaskets for doors and windscreens. Accordingly they play an important role not only in the mentioned branch. In this contribution, we investigate a compressible cellular rubber in an uniaxial tension test under quasi-static and isothermal conditions. From the modelling site, we introduce a continuum mechanical material model on the basis of the theory of porous media which is able to describe the complex compressible material behaviour of the tested specimen. The established material parameters are identified by a biologic evolution strategy method and the simulations are compared with the obtained experimental results.

Application of Rosenbrock-type methods to a constitutive model of polymeric material. **Ahmad-Wahadj Hamkar** (Universität Kassel, Germany), Stefan Hartmann (Universität Kassel, Germany) GA/CT2384/006

Polymeric materials show a pronounced time dependent material behaviour like relaxation and creep. In the case of polyoxymethylene this is also combined with a tension-compression asymmetry. Furthermore, there are indications of remaining deformations so that a constitutive model of viscoplasticity is an appropriate choice. Overstress-type models have an additional advantage in view of there modular structure whereas a yield-function free concept is more suitable. Based on a constitutive model presented in [1] the structured behaviour of parts has to be computed. Commonly, iteration-based implicit finite element computations are applied. In this lecture, linear-implicit Runge-Kutta methods (Rosenbrock-type method) are applied to the system of differential-algebraic equations resulting from the space discretisation by means of finite elements. This has the essential advantages that time-adaptivity is applicable. Moreover, there are neither global nor local iteration procedures. The lecture shows the behaviour of the new global finite element approach and compares it to classical implicit (iterative) procedures. [1] Hartmann, S.: A thermomechanically consistent constitutive model for polyoxymethylene: experiments, material modeling and computation, currently published online Archive of Applied Mechanics 2006

Modelling of mechanical twinning on the microscale. **Rainer Glüge** (Universität Magdeburg, Germany) GA/CT5062/006

Since magnesium and its alloys have been rediscovered as adequate materials for lightweight-structures, there is an increased interest in an accurate modeling of the plastic material behavior. At room temperature, mechanical twinning is an important deformation mode, which influences strongly the material properties, especially the crystallographic texture and the grain morphology. There exist some material models that incorporate mechanical twinning from a macroscopic point of view in a statistical and homogenized sense, while material models that are able to predict the twin formation on the microscale are object of ongoing research, which is due to the phase-transition character of twinning. The latter type of models is predestined to be combined with the representative volume element technique. Such approach should allow a much more precise prediction of the microstructure evolution than a statistical model. In this talk, a short comparison of some micro-models is given. Then, a modeling technique that uses a nonconvex elastic potential and the special characteristics that emerge in conjunction with mechanical twinning are discussed in detail.

GA/CTS4457/06: Ferroelasticity and other topics in materials science.

Organiser: Franz-Joseph Barthold (Universität Dortmund, Germany)
Co-organiser: Alexander Lion (Universität der Bundeswehr, Germany)
Co-organiser: Rolf Mahnken (Universität Paderborn, Germany)

On the modelling of rate-dependent ferroelastic switching. **Andreas Menzel** (Universität Siegen, Germany), Arunachalakasi Arockiarajan (IIT Madras, India), Srinivasan M Sivakumar (IIT Madras, India) GA/CT1939/006

Piezoelectric materials, which are nowadays widely used for smart materials and intelligent systems applications, possess severely nonlinear response under high loading conditions. Such effects, as monitored by representative hysteresis and butterfly curves, stem from phase-transformations of the underlying polycrystalline microstructure. So-called spontaneous polarisation as well as spontaneous strains thereby take place of the level of individual grains or rather domains.

To account for such effects within a finite-element-based modelling approach, an energy-related switching criterion is adopted, whereby, at this stage, we restrict ourselves to ferroelasticity. In this regard, domain switching is initiated as soon as the corresponding reduction in energy exceeds a particular threshold. On the one hand, microstructural characteristics are directly incorporated by adapting the underlying (local) elastic properties, while, on the other hand, also the format of the spontaneous strains reflects the geometry of the assumed tetragonal unit-cells. Rate-dependent response, however, is phenomenologically introduced my means of a Weibull probability function weighting the switching threshold.

With this framework in hand and based on a staggered iteration technique embedded into a three-dimensional finite element formulation, numerical simulations recover representative hysteresis and butterfly curves, whereby use of randomly initialised unit-cells as well as of volume averaging techniques is made.

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Contact area of solid bodies: calculations compared to measured results. **Jan-Hinrich Sick** (TU Braunschweig, Germany), Georg Ostermeyer (TU Braunschweig, Germany) GA/CT2339/006

A novel attempt is made to directly measure the contact area of solid bodies by relating it to the electrical contact resistance. This method was used by F. P. Bowden and D. Tabor in the 1930s already. We confined the setup by use of low conductive thin film coatings. This way it is possible to point out the influence of contact area in contrast to incidental contaminations. By use of wear resistant coatings it is possible to measure the contact area in sliding contacts as well. We compare new measurements to predictions of contact area calculated on base of recent models like the discrete Greenwood and Williamson model proposed by M. Ciavarella, V. Delfine and G. Demelio (2006). This project is supported by the German Research Foundation.

An evolution model in contact mechanics with dry friction. **Florian Schmid** (Weierstraß-Institut Berlin, Germany) GA/CT2464/006

We present an existence result for an evolution problem in contact mechanics with dry friction. Our physical model consists of an elastic system whose shape is determined by the position of N single particles, thus leaving only 3N degrees of freedom. You may think of N particles that are linked by nonlinear elastic springs. The whole system will be driven by external forces which we assume to evolve quite slowly in time. This will allow us to neglect inertia terms in the model. Further we assume a rigid plane to be given which cannot be penetrated by any particle. As soon as a particle comes into contact with the plane friction will occur which will be modelled using Coulomb's friction law.

Mathematically this leads us to a highly nonlinear and rate-independent problem with two severe difficulties. The first arises from the frictional term which is usually written as a multivalued functional. The second difficulty is due to the change from contact to non-contact of each particle. We are going to present an energetic formulation for such a problem and a time incremental method to prove existence. The method is such that it overcomes both difficulties at once.

Description of inelastic deformation of solids accounting for shear banding. **Ryszard Pecherski** (Cracow University of Technology, Poland) GA/CT4813/006

The subject of the study are ultra fine grain (ufg) and nanocrystalline metals (nc-metals). Experimental investigations of the behaviour of such materials under quasistatic as well as dynamic loading conditions related with microscopic observations show that in many cases the dominant mechanism of plastic strain is multiscale development of shear deformation modes - called usually shear banding. The comprehensive discussion of these phenomena is given e.g. in [1]. Our objective is to propose a new description of inelastic deformation, which accounts for the observed mechanism of shear banding. The shear banding contribution function, which was introduced formerly in [2], [3] and applied in continuum plasticity accounting for shear banding in [4], [5] plays pivotal role in the proposed description. The derived constitutive equations were identified and verified with application of available experimental data. The possibilities of the application of the proposed descrip-

tion for modelling of plastic flow of hard deformable and high strength materials are discussed.

1. M.A. Meyers, A. Mishra, D.J. Benson, Mechanical properties of nanocrystalline materials, Progr. Mater. Sci., 51, 427-556, 2006. 2. R.B. Pecherski, Modelling of large plastic deformation produced by micro-shear banding, Arch. Mech., 44, 563-584, 1992. 3. R. B. Pecherski, Macroscopic effects of micro-shear banding in plasticity of metals, Acta Mechanica, 131, 203-224, 1998. 4. R.B. Pecherski, K. Korbel, Plastic strain in metals by shear banding. I. Constitutive description for simulation of metal shaping operations, Arch. Mech., 54, 603-620, 2002. 5. Z. Nowak, R.B. Pecherski, Plastic strain in metals by shear banding. II. Numerical identification and verification of plastic flow, Arch. Mech., 54, 621-634, 2002.

GA/CTS4450/06: Plasticity, visco-plasticity and damage.

Organiser: Markus Böl (TU Braunschweig, Germany)
Co-organiser: Alexander Lion (Universität der Bundeswehr, Germany)
Co-organiser: Rolf Mahnken (Universität Paderborn, Germany)

Comparison of two integration algorithms for finite plasticity combined with nonlinear kinematic and isotropic hardening at the example of springback. **Michael Pietryga** (TU Braunschweig, Germany), Stefanie Reese (TU Braunschweig, Germany) GA/CT2258/006

In this research a large-deformation elastic-visco-plastic model with non-linear kinematic and non-linear isotropic hardening is implemented. The model is capable of describing cyclic hardening and the Bauschinger effect, which are very important for the modelling of springback in sheet metal forming. The model is derived from a thermomechanical framework and is based on the multiplicative split of the deformation gradient. A major topic of this talk is the comparison of two implicit time integration schemes: 1) a new version of the exponential map algorithm [1] and 2) a modification to the classical backward Euler method (see for earlier concepts [2]). Both algorithms fulfill plastic incompressibility. Some aspects, such as the necessity to fulfill plastic incompressibility, several possibilities to modify the classical backward Euler method in order to fulfill plastic incompressibility, or the numerical efficiency of both algorithms, are discussed. The comparison of the methods is performed at the material point level as well as at the structural level. For this purpose, the FE analysis tool ABAQUS is used. The applicability of the presented model at the structural level is demonstrated for the case of springback prediction in sheet metal forming simulations. [1] D. Christ, S. Reese, Is it necessary to model shape memory alloys within the scope of large strains?, Proceedings of SPIE: Smart Structures and Materials, Ed.: W.D. Armstrong, Volume 6170, San Diego, USA (2006), 247-257 [2] C. Miehe, Multisurface Thermoplasticity for single crystals at large strains in terms of eulerian vector updates, Int. J. Solids Structures, Vol. 33, No. 20-22, pp. 3103-3130, 1996

A non-local extension of the Gurson–Tvergaard–Needleman damage model for the simulation of metallic structures. **Christian Fell** (TU Darmstadt, Germany) GA/CT2452/006

The present contribution is based on a non-local extension of the model of Gurson-Tvergaard-Needleman (GTN) for ductile damage [1]. The formulation applies a multiplicative decomposition of the deformation gradient and is valid for finite plastic deformation. In order to avoid mesh dependencies of the finite-element solution a gradient-enhanced model for regularization is applied. Here, we use the gradient of the damage variable in terms of the void fraction, cf [3]. The model is able to describe void nucleation, growth and coalescence. In the original work [2] the coalescence is modeled by a bilinear relation between void fraction and modified void fraction. Opposed to this we propose a smooth relation between these quantities, which is realized by means of a higher order polynomial. Representative numerical examples serve to verify the numerical features and to validate the modelling.

[1] A. L. Gurson: Continuum theory of ductile rupture by void nucleation and growth, J. Engrg. Mat. Tech., 99 (1977) 2–15.
[2] V. Tvergaard, A. Needleman: Analysis of the cup-cone fracture in a round tensile bar, Acta metall., 32 (1984) 157–169.
[3] F. Reusch, B. Svendsen, D. Klingbeil: Local and non-local Gurson-based ductile damage and failure modelling at large deformation, Eur. J. Mech. A/Solids 22 (2003) 779Ű-792.

On the convergence of kinetic variational inequality to quasi-static variational inequality with applications to the elastoplasticity. **Adrien Petrov** (WIAS, Germany) GA/CT2432/006

We prove a priori bounds for the dynamic elastic–plastic systems that lead to the convergence to the quasi-static case. The discussion of convergence is preceded by the presentation of mathematical formulations, existence and uniqueness results for those dynamic and quasi-static problems.

Numerical analysis of shear-bands in solids by means of computational homogenization. **Lidija Stankovic** (Ruhr-Universität Bochum, Germany), Jörn Mosler (Ruhr-Universität Bochum, Germany) GA/CT2748/006

A novel fully three-dimensional framework for the numerical analysis of shear bands in solids undergoing large deformations is presented. The effect of micro shear bands on the macroscopic material response is computed by means of a homogenization strategy. More precisely, a strain-driven approach which complies well with displacement-driven finite element formulations is adopted. The proposed implementation is based on periodic boundary conditions for the micro-scale. Details about the implementation of the resulting constraints into a three-dimensional framework are discussed. The shear bands occurring at the micro-scale are modeled by a cohesive zone law, i.e., the tangential component of the traction vector governs the relative shear sliding displacement. This law is embedded into a Strong Discontinuity Approach (SDA). To account for realistic sliding modes, multiple shear bands are allowed to form and propagate in each finite element.

3D continuum mechanical modeling of the Portevin–Le Châtelier effect. **Gèza Bondàr** (Universität Karlsruhe (TH), Germany), Thomas Böhlke (Universität Karlsruhe, Germany), Juri Estrin (TU Clausthal, Germany) GA/CT2678/006

In many Al-, Cu-, Fe- and Ni-based alloys jerky flow associated with the Portevin–Le Châtelier (PLC) effect appears within a specific range of temperature and strain rate. This effect which reduces the ductility and the surface quality of sheet materials is caused by the interaction of free dislocations with obstacles (Estrin, 1987). A three dimensional continuum mechanical model concerning the dynamic strain ageing is presented. A comparison of the predictions of the three dimensional model with experimental results is given. Special emphasis is given to the determination of the instability region in the strain and strain-rate space (Kubin and Estrin, 1990).

Estrin, J. (1987). Stoffgesetze der plastischen Verformung und Instabilitäten des plastischen Fließens. VDI Forschungsheft 642, 1-48.

Kubin, L.P. and Estrin, Y. (1990). Evolution of dislocation densities and the critical conditions for the Portevin-Le Chatelier effect. Acta metall. mater. 38(5), 697-708.

GA/CTS4458/06: Sensitivity, identification and simulation.

Organiser: Serdar Göktepe (Universität Stuttgart, Germany)
Co-organiser: Alexander Lion (Universität der Bundeswehr, Germany)
Co-organiser: Rolf Mahnken (Universität Paderborn, Germany)

Aspects of shape and parameter sensitivity analysis in the theory of porous media. **Franz-Joseph Barthold** (Universität Dortmund, Germany), Jörg Stieghan (TU Braunschweig, Germany) GA/CT3112/006

This contribution is concerned with the application of variational shape sensitivity analysis and parameter sensitivity analysis to the theory of porous media. Both areas contribute to structural optimization and inverse problems like parameter identification. The correct and efficient derivation, implementation and computation of the sensitivities, i.e. the gradient values of objectives and constraints with respect to different kind of design variables, have an significant influence on the overall performance of the nonlinear programming algorithms applied to the numerical treatment of inverse problems.

The theory of porous media is build upon the mixture of several phases and their interaction. Thus, a complex continuum mechanical description for each single phase as well as for the micture is used in this approach. This proposal formulates a general viewpoint using local coordinates which permit a rigorous split of continuum mechanical functions into parts being either geometry or deformation dependent.

The variational approach to sensitivity analysis is build upon this separation and yields some general inside into the structure of porous media. Especially, the significance of the material parameters of each single phase as well as the mixture ratio for the overall deformation behavior can be quantified. We will summarize our research of the theoretical and computational treatment by means of selected examples considering soil mechanics as well as foams.

Granular materials: parameter identification and modelling of localization problems. **Okan Avci** (Universität Stuttgart, Germany), Wolfgang Ehlers (Universität Stuttgart, Germany) GA/CT3988/006

The prediction of landsliding requires an exact knowledge of the mechanical behaviour of granular materials. This kind of materials, e. g., sand, have a very complex deformation behaviour, which depend on the stress-state and the loading history. Via homogeneous triaxial tests on dry sand specimens, the material behaviour of the grain structure can be characterized. Additionally, an appropriate elasto-plastic material law to describe the solid skeleton in the frame of *Theory of Porous Media* (TPM) is used, which is implemented in the FE tool PANDAS. Furthermore, a single-surface yield criteria with isotropic hardening, which limits the elastic domain, and non-associated plastic flow is assumed.
The determination of the material parameters of the linear elasticity law as well as the single-surface yield criteria based on test data of triaxial experiments is done with a derivative based optimization method (donlp2), which is coupled with PANDAS. Finally, a simulation of a benchmark test is presented to show shear band localization effects. In this case, the material behaviour is described by a triphasic porous media model based on the TPM, where the single constituents are a deformable solid skeleton and two pore fluids, i. e., pore water and pore air.

Adaptive modeling and simulation of shear banding and high speed. **Christian Hortig** (Universität Dortmund, Germany), Bob Svendsen (Universität Dortmund, Germany) GA/CT2137/006

High speed cutting is a process of high interest in modern production engineering. Besides the advantage of high productivity as a result of the increase of cutting speed, a decrease of cutting forces can be observed. In order to take advantage of the potential of the high speed cutting process, the knowledge of the working mechanisms in combination with the material behavior is essential. Experimental observations detect the occurrence of localized adiabatic shear bands as the main mechanism of deformation of chip formation. These shear bands develop in localized areas of temperature dependent softening, surrounded by material in a process of strain and strain rate dependent hardening. The fact of high deformation rates and the mechanism of localized shear bands forces the implementation of a temperature and rate dependent material model which will be discussed. The strong mesh dependence of the phenomenon of localized shear banding is one of the key problems in the context of FE simulation of the high speed cutting process, as orientation and characteristic length of the mesh force direction respectively expansion of localization. It will be shown that the influence of the orientation of the mesh can be reduced by using adaptive procedures with the aim to reduce the characteristic element length locally. Here, a Python environment is used to connect the different components of the adaptive procedure, consisting of the error estimator, the mesh generator, the mapping procedure and the solver. The adaptive procedure will be discussed in detail. Besides a reduced mesh dependence, using adaptive remeshing enables a more realistic modeling of the separation of the chip and the resulting surface. Up to this point the presented simulation results are restricted to the 2D case. The pathological mesh dependence and thus the characteristic element edge length forces the width of the material instability. Thus an additional information is required to give a physical description of the width of the material instability. Here the formulation of a non local plasticity model is favored and implemented. Simulation results will be presented.

Boundary-value problems in the theory of binary mixtures. **Merab Svanadze** (Ilia Chavchavadze State University, Georgia) GA/CT615/006

Great strides have been made in developing a theoretical basis for studying the mechanics of mixtures starting with the pioneering work of Truesdell and Toupin (1960). The mathematical models of the binary mixtures of elastic and thermoelastic solids are presented by Green and Naghdi (1965), Steel (1967), Lempriere (1969), Bedford and Stern (1970), Filippov (1971), Rushchitski (1978), McNiven and Mengi (1979), Khoroshun and Soltanov (1984), and Iesan (1997).

In this paper a wide class of the boundary value problems of the linear theory of binary mixtures of elastic and thermoelastic solids is investigated by means of the boundary integral method (BIM). The fundamental solutions of the equations of steady oscillations for mathematical models of the binary mixtures are constructed in terms of elementary functions.

The uniqueness and existence theorems of solutions of the interior and exterior boundary value problems by means BIM

and multidimensional singular integral equations are proved. The Sommerfeld-Kupradze type radiation conditions are established.

The existence of eigenfrequencies of the interior homogeneous boundary value problems of steady oscillations is studied. The basic properties of wave numbers are treaded. The connection between plane waves and eigenfrequencies is established. The formula of asymptotic distribution of eigenfrequencies is obtained.

Boundary-value problems of the theory of heat propagation in a binary mixture. **Maia Svanadze** (Tbilisi State University, Georgia) GA/CT844/006

The linear mathematical models of heat propagation in a binary mixture are presented by Gurtin and De La Penha (1970), Khoroshun and Soltanov (1984), Iesan (1997).

In this paper the boundary value problems of steady oscillations of the linear theory of heat propagation in a binary mixture are investigated. The fundamental solution of the system of the equations of steady oscillations is constructed in terms of elementary functions. A solution of Galerkin type is established. The integral representation of Somigliana type for the regular vectors is presented. The basic properties of single-layer, double-layer and volume potentials are studied. The uniqueness and existence theorems of solutions of the interior and exterior boundary value problems by means boundary integral method (potential method) are proved.

GA/CTS4451/06: Anisotropic materials.

Organiser: Stefan Hartmann (Universität Kassel, Germany)
Co-organiser: Alexander Lion (Universität der Bundeswehr, Germany)
Co-organiser: Rolf Mahnken (Universität Paderborn, Germany)

On the construction of anisotropic polyconvex energy densities. **Vera Ebbing** (Universität Duisburg-Essen, Germany), Jörg Schröder (Universität Duisburg-Essen, Germany), Patrizio Neff (TU Darmstadt, Germany) GA/CT2365/006

In order to guarantee the existence of solutions in large strain elasticity, the free-energy function has to be quasiconvex. This condition is rather complicated to handle. Therefore, polyconvex functions which are always quasiconvex are usually considered, see [1]. For isotropic materials, there exists a wide range of constitutive functions that satisfies the polyconvexity requirement. In this talk we discuss the formulation of anisotropic polyconvex free energy functions in a coordinate-variant setting. A variety of polyconvex energy densities in a transversely isotropic and orthotropic coordinate-invariant framework has been proposed in [2,3]. The goal of the talk is the construction of constitutive functions in terms of the elements of a local functional basis which automatically satisfy the polyconvexity condition. The local functional basis is considered in a preferred frame and consists of terms of the right Cauchy-Green tensor. After giving a general introduction we focus on several model problems and present some numerical examples.

[1] Ball, J.M., Convexity Conditions and Existence Theorems in Non-Linear Elasticity, Archive of Rational Mechanics and Analysis, 63, 337-403, 1977

[2] D. Balzani, Polyconvex Anisotropic Energies and Modeling of Damage Applied to Arterial Walls, PhD-Thesis, Scientific Report of the Institute of Mechanics, University of Duisburg-Essen, Verlag Glückauf Essen (2006)

[3] J. Schröder and P. Neff, Invariant Formulation of Hyperelastic Transverse Isotropy Based on Polyconvex Free Energy Functions, Int. J. Sol. Struct. 40, 401-445 (2003)

Polyconvex energy densities with applications to anisotropic thin shells. **Daniel Balzani** (Universität Duisburg-Essen, Germany), Jörg Schröder (Universität Duisburg-Essen, Germany), Friedrich Gruttmann (TU Darmstadt, Germany) GA/CT1872/004

The numerical framework for the simulation of anisotropic thin shells is presented by using polyconvex strain energy functions. The nonlinear shell theory is based on the Reissner-Mindlin kinematic along with inextensible director vectors and enhanced assumed shell strains are considered, cf. [1]. For the variational framework we consider a three field variational functional taking into account independent displacements, enhanced strains and stress resultants, where the latter field is eliminated applying some orthogonality conditions. The iterative fulfillment of the zero normal stress condition at the integration points allows consideration of arbitrary three-dimensional constitutive equations. Thus the developed four-node shell element with 5 or 6 nodal degrees of freedom can account for finite deformations. For the representation of the anisotropy we use the concept of structural tensors and formulate the strain energy function in terms of the principal and mixed invariants of the right Cauchy-Green tensor and the structural tensor. Due to the fact that we are interested in fiber-reinforced materials we consider an additive structure of the energy decoupled into an isotropic part for the matrix and a superposition of transversely isotropic parts for the fiber families. In order to guarantee the existence of minimizers *a priori* and additionally satisfy the quasiconvexity- and Legendre-Hadamard condition, we focus on polyconvex strain energy functions as proposed in [2], see also [3]. Numerous numerical examples show the anisotropy effect by comparing isotropic shells with anisotropic ones.

[1] D. Balzani, F. Gruttmann, J. Schröder, Analysis of Thin Shells using Anisotropic Polyconvex Energy Densities, in preparation

[2] D. Balzani, Polyconvex Anisotropic Energies and Modeling of Damage Applied to Arterial Walls, PhD-Thesis, Scientific Report of the Institute of Mechanics, University of Duisburg-Essen, Verlag Glückauf Essen (2006)

[3] J. Schröder and P. Neff, Invariant Formulation of Hyperelastic Transverse Isotropy Based on Polyconvex Free Energy Functions, Int. J. Sol. Struct. 40, 401-445 (2003)

Stability of elastic composite materials having a negative-stiffness phase. **Dennis Kochmann** (Ruhr-Universität Bochum, Germany), Walter Drugan (University of Wisconsin, USA) GA/CT1911/006

Composite materials theory limits the attainable overall elastic moduli of a composite in terms of the properties of its constituents, presuming positive-definiteness (positive stiffness) for each constituent to ensure overall stability. Admittance of a negative-stiffness phase, however, facilitates the composite material to strongly exceed these well-known bounds. Recent experimental results give evidence for this behavior and exhibit bound-exceeding performance. However, no analytical investigation has been reported to prove overall stability for such a composite material.

An analytical method is established to derive the admissible ranges, for dynamic overall stability, for the elastic moduli of homogenous, isotropic linear-elastic bodies with arbitrary geometry and boundary conditions. This method is confirmed for two-dimensional circular geometries by proving the requirements of positive-definiteness (for a body with pure traction

boundary conditions) and strong ellipticity (for pure displacement boundary conditions). This approach at hand, it is feasible to derive stability bounds on the elastic moduli for any set of geometry and boundary conditions.

A two-dimensional (plane strain) model of a two-phase composite material is employed to obtain restrictions on the elastic moduli of a composite consisting of a coated circular-cylindrical inclusion. Our general results are simplest to interpret in the case of a thin coating. In this case, our results show that the inclusion may indeed violate positive-definiteness (within the range of strong ellipticity), given a coating with sufficiently stiff elastic moduli (satisfying a restriction stronger than positive-definiteness), while retaining overall stability of the composite. Therefore, a negative stiffness inclusion can be stabilized by a sufficiently stiff coating. This approach may give rise to novel advances into composite materials with superior performance.

Modeling dissipative effects in anisotropic materials by means of evolving generalized structural tensors. **Alexander Ehret** (RWTH Aachen, Germany), Mikhail Itskov (RWTH Aachen, Germany) GA/CT2943/006

Structural tensors are a practical means to describe anisotropic properties of a material. They allow to define the symmetry group of the material and finally to incorporate anisotropic behavior into constitutive models. Recently, polyconvex anisotropic hyperelastic models were proposed which are based on linear combinations of the structural tensors referred to as generalized structural tensors. The corresponding non-negative components represent weight factors of the preferred material directions and are considered as material constants of the constitutive model. In the present contribution, these weight factors and consequently the generalized structural tensors are allowed to change in order to describe evolving material properties. This approach enables to account for dissipative effects in anisotropic materials like e.g. softening or the so-called preconditioning, which is experimentally observed in biological soft tissue samples during early load cycles. Applying the theory of internal variables, the relevant thermodynamic quantities are derived, suitable yield conditions are discussed and appropriate evolution equations are suggested. As a numerical example, the preconditioning behavior of soft tissue samples is considered.

Cyclic martensitic phase transformation of monocrystals with finite strains. **Gautam Sagar** (Universität Hannover, Germany), Erwin Stein (Universität Hannover, Germany) GA/CT2312/006

Based on BainŠs principle, a C^1-continuous thermo-mechanical micro-macro constitutive model for monocrystals with finite strains and hyperelastic free energy function is used. It is represented by a unified non-convex Lagrangian variational functional including phase evolution equations with mass conservation and quasi-convexification during phase transformation processes. The convexification problem is solved here by generalizing the explicit form of the lower Reuss bound for small strains given by Govindjee, Mielke and Hall (2003) to finite strains. Iterative time integration of the evolution equation is programmed in C++ and implemented into the UMAT-interface of the finite element package Abaqus for the current configuration associated with Jaumann rate. The validation of this phase transformation model is carried out for both quasiplastic and superelastic effects of $Cu_{82}Al_{14}Ni_4$ monocrystals with experimental data supplied by Xiangyang et al. (2000). Computations are done using 3D-hexahedral B-bar elements. The numerical results give good agreement with experimental values. An interesting result of numerical simulation is the local average behavior of *yield tooth* pattern (measured zig-zag curves) which could not be represented by linear theory.

On the implicit standard material model. **Michael Ban** (RWTH Aachen, Germany), Dieter Weichert (RWTH Aachen, Germany) GA/CT2335/006

The Implicit Standard Material (ISM) model, introduced by de Saxcé, is an extension of the Generalized Standard Material model. The ISM model allows to analyze coupled and non-associated constitutive laws of potential type. The mathematical framework is based on separately convex functionals, called bipotentials. In our presentation, we focus on variational methods for the ISM model and applications to shakedown theory.

GA/CTS4572/06: Viscoelasticity.

Organiser: Jörn Ihlemann (Deutsches Institut für Kautschuktechnologie, Germany)
Co-organiser: Alexander Lion (Universität der Bundeswehr, Germany)
Co-organiser: Rolf Mahnken (Universität Paderborn, Germany)

Comparative analysis of viscoelastic models involving fractional derivatives of different orders. **Marina Shitikova** (Voronezh State University, Russian Federation), Yuriy Rossikhin (Voronezh State University, Russian Federation) GA/CT863/006

In the given paper, a comparative analysis of the models involving fractional derivatives of different orders is given. Such models of viscoelastic materials are widely used in various problems of mechanics and rheology.

In particular, it is shown the equivalence of the model presented by Koeller (1984)

$$\sum_{i=1}^{n} a_i D^{i\alpha}\varepsilon = \sum_{j=1}^{n} b_j D^{j\alpha}\sigma, \qquad (1)$$

and the model proposed by Rabotnov (1966)

$$\varepsilon = J_\infty \left[\sigma + \sum_{i=1}^{n} g^i \ni_\alpha^* (-\tau_i^{-\alpha})\sigma\right], \qquad (2)$$

where $D^{i\alpha}\varepsilon$ and $D^{j\alpha}\sigma$ are Riemann-Liouville fractional derivatives of the strain and stress, respectively, a_i, b_j, g_i, and τ_i are given values, $0 < \alpha < 1$ is the order of the fractional derivative, J_∞ is the instantaneous compliance, the operator

$$\ni_\alpha^* (-\tau_i^{-\alpha})\sigma = \int_0^t \ni_\alpha (-t'/\tau_i)\sigma(t-t')dt',$$

and the fractional exponential function

$$\ni_\alpha (-1, t'/\tau_i) = \frac{t^{\alpha-1}}{\tau_i^\alpha} \sum_{n=0}^{\infty} (-1)^n \frac{(t/\tau_i)^{\alpha n}}{\Gamma[\alpha(n+1)]}$$

goes over into an ordinary $\exp(-t/\tau_i)$ at $\alpha = 1$ ($\Gamma[\alpha(n+1)]$ is the gamma-function).

Inverse of the Rabotnov's model (2) is carried out, and it is shown how to apply it for approximation of hereditary kernels determined experimentally.

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Representation of the linear viscoelastic behaviour of wood with a constitutive theory based on fractional time derivatives. **Thomas Ranz** (Universität der Bundeswehr München, Germany) GA/CT3620/006

Like many other materials used in mechanical and civil engineering, wood shows a pronounced history-dependent mechanical material behaviour. Due to its anisotropy its rheological behaviour is strongly dependent on the direction. In this research project, the material behaviour is represented with a phenomenological theory of anisotropic fractional viscoelasticity. In order to identify the material functions and parameters, the time-dependent creep compliances are measured in three orthogonal directions under tension and shear. As a result of the developed constitutive approach, the experimentally observed creep data is described by several power functions. In the second part of the presentation, some differences between classical models of viscoelasticity which are based on Kelvin-Voigt or Maxwell elements and the fractional approach are presented. The assets and drawbacks with respect to wood are discussed.

Critical remarks on finite multiplicative visco-elasticity and formulation of finite fractional visco-elasticity. **Alexander Lion** (Universität der Bundeswehr, Germany) GA/CT1307/006

A critical consideration of the theory of finite multiplicative viscoelasticity splitting the deformation gradient into a set of elastic and inelastic parts in parallel and introducing corresponding intermediate configurations is given. If different intermediate configurations are taken in parallel, this approach leads to a set of nonlinear evolution equations for the inelastic deformation tensors and corresponds to a generalization of discrete relaxation spectra to finite strains. Since there is no internal variable-free formulation of this approach its generalization to continuous spectra or to a fractional derivative-based theory of finite viscoelasticity is not possible. To this end, a different formulation of finite viscoelasticity is discussed: it is formulated without any split of the deformation gradient, includes discrete as well as continuous relaxation spectra and can easily be used to formulate a fractional derivative-based theory of finite viscoelasticity. The most simple model of this type corresponds to the well-known springpot of one-dimensional fractional viscoelasticity and interpolates between the Mooney Rivlin model of finite elasticity and the model of the linear viscous fluid. This model leads to a relaxation behaviour of the power-law type, but more complicated models of this type lead to a relaxation behaviour which is given by Mittag–Leffler functions.

3D finite-element modeling of polymeric materials with C^1-continuous elements. **Paul Fischer** (TU Kaiserslautern, Germany), Ellen Kuhl (TU Kaiserlautern, Germany), Paul Steinmann (TU Kaiserslautern, Germany) GA/CT2262/006

Motivated by recent development in compound polymeric materials, we aim to model microfibrillar polymer-polymer composites. This can be accomplished in two different ways, macroscopic phenomenologically or microscopically-motivated. Here, we followed the latter approach. To this end, entropy elastic chain models like the Langevin model are embedded in various kinds of representative unit cells. This provides a constitutive model for the material. The finite element method with the classical Jacobian-pressure formulation is most common to avoid locking and other numerical instabilities. In the recent literature an alternative strategy based on a single field 3D Hermitian element with C1 interelement continuity of the displacements has been suggested. The fundamental advantage of these elements is a continuous stress interpolation. Numerical examples will demonstrate their improved convergence properies as compared to classical mixed finite elements.

Measurement of the elastoplastic strain at the crack tip on the specimen. **Yuri Lapusta** (Institut Français de Méchanique Avancée, France), Petro Yasniy (Ternopil State Ivan Pulu'j Technical University, Ukraine), Yuriy Pyndus (Ternopil Ivan Pul'uj State Technical University, Ukraine), Ihor Shulgan (Ternopil State Technical University, Ukraine) GA/CT4132/006

An experimental technique for study of the elastoplastic strain at the crack tip is proposed. It deals with the determination of the elastoplastic displacements of the material on the plane center cracked panel surface and the identification of the elastoplastic deformations at the crack tip using an improved method of coordinate grids. The technique uses chemical etching of a grid (100 dots per mm2) with constant step gradation on the specimen surface. The point diameter approximately equals 0.02 mm. Phototype-setting device Scitex-Dolev4pressVEG750 (resolution 4064 dots per inch) is used to prepare the grid phototemplate (negative). The depth of grid holes is 2-3 micrometers. Such grid has a good resistance to high strains including high temperature. It has high accuracy, contrast and constant step. The digital images of specimen surface at the crack tip before loading and at the maximum tensile load and after unloading were obtained. To photograph the coordinate grid, a binocular microscope (magnification factor - 70x), a digital camera Sony (Carl Zeis optics) with resolution (6 Megapixels) and some illuminating equipment were used. A program for the calculation of coordinate grid points displacement was developed. This program is based on a bit-by-bit coordinate grid points digitalization, an automated determination and identification of the grid points center coordinates on the virgin and deformed material pictures, and on calculation of their displacement and strain. Stress-strain state at the crack tip under similar loading conditions was carried out using FEM. The plane stress state was considered. The calculations were carried out for a uniaxial loading of center cracked panel of aluminium alloy D16chT (analogue of American 2024T3). A comparison of the elastoplastic and plastic strains at the crack tip calculated using the FEM and using the grids method was performed.

GA/CTS4454/06: Ferro-electric and shape-memory materials.

Organiser: Alexander Lion (Universität der Bundeswehr, Germany)
Co-organiser: Rolf Mahnken (Universität Paderborn, Germany)

Ferroelektriosche Piezokeramiken: Experimente, Mikromechanik, Materialmodelle und Finite Elemente Analyse. **Marc Kamlah** (Forschungszentrum Karlsruhe, Germany) GA/CT3607/006

Dies ist ein von Prof. A. Lion eingeladener Beitrag in der Sektion Materialtheorie.

Koautoren: B. Laskewitz und D. Zhou

Abstract: Die wichtigste Materialklasse fuer die Ausnutzung des piezoelektrischen Effektes, der zunehmende Bedeutung in Aktorik und Sensorik besitzt, sind ferroelektrische Keramiken. In diesem Vortrag stellen wir zunaechst die mikroskopische Struktur des Materials mit Domaenen und Umklappprozessen vor. Sodann diskutieren wir ein mikromechanisches Volemenelement. Weiterhin werden ein phaenomenlogisches und ein mikroskopisch motiviertes Materielmodell vorgestellt. Schliesslich betrachten wir die Anwendung dieser Modelle in der Finiten Elemente Analyse von Polungsprozessen in piezokeramischen Komponenten.

Simulation of asymmetric effects for shape-memory alloys. **Stefan Wilmanns** (Universität Paderborn, Germany), Rolf Mahnken (Universität Paderborn, Germany) GA/CT1683/006

Extended experimental tests for shape memory alloys exhibit different behaviours for different loading types, such as tension, compression and shear. These observations, labelled here briefly as asymmetric effects, are reported in the literature; e.g., in [1] or [2]. The paper is concerned with modelling of these effects in the framework of plasticity. To this end an additive decomposition of the flow rule is assumed into a sum of weighted stress mode related quantities. The characterization of the stress modes is obtained in the octahedral plane of the deviatoric stress space in terms of a single scalar variable, such that stress mode dependent scalar weighting functions can be constructed. Furthermore the numerical implementation into a finite element program of the resulting set of constitutive equations is outlined. For parameter identification a sequential strategy exploiting the mode decomposition and the individual loading scenarios, such as tension, compression and shear, respectively is described. Verification of the proposed methodology is succeeded for simulation of the pseudoelastic behaviour of shape memory alloys with different hardening characteristics in tension and shear.

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Keywords: Shape memory alloys, tension, compression, shear, asymmetry, constitutive equations, finite-element simulation, parameter identification

Thermo-mechanical behavior of pseudo-elastic NiTi *shape-memory alloys.* **Patrick Luig** (Ruhr-Universität Bochum, Germany), Christian Grabe (Ruhr-Universität Bochum, Germany), Otto Bruhns (Ruhr-Universität Bochum, Germany) GA/CT2376/006

The thermomechanical behavior of polycrystalline Ni-rich pseudoelastic NiTi shape memory alloys is analyzed. Special focus is on regions within the stress strain diagram which are regarded as linear elastic in common phenomenological material models, i.e. the region between zero stress and the beginning of the pseudoelastic plateau as well as the region within the hysteresis. In both cases, severe temperature changes can be observed. A possible explanation for this effect is twofold: On the one hand, it might be explained by the presence of an R-phase transformation. On the other hand, self-accommodated martensite of the B19' phase may form. However, the assumption of a purly linear elastic material behavior in those regions does not seem to hold true in general.

A new method for the simulation of shape-memory polymers. **Markus Böl** (TU Braunschweig, Germany), Stefanie Reese (TU Braunschweig, Germany) GA/CT1971/006

Shape memory polymers belong to the group of smart materials that can be easily formed into complex shapes, retaining memory of their original shape even after undergoing large deformations. This characteristic makes the material interesting for medical application fields. Here it is used as stent or suture material, where the memory effect is controlled by the temperature of the body. The shape memory properties can be quantified by cyclic thermomechanical investigations. One cycle includes the "programming" of the specimen and the recovery of its permanent shape. In a typical test program the specimen is stretched up at room temperature to a certain stretch λ_{m}. The sample is then cooled at constant stretch λ_{m}. If the transition temperature is reached the shape of the sample is fixed. After reheating to the transition temperature the sample is contracting itself and the original shape is restored. For the simulation of such material behaviour under varying thermal and mechanical conditions while the polymer undergoes large deformations we present an innovative finite element model which incorporates the micro structure of rubber-like material.The proposed approach is based on a so-called unit cell consisting of one tetrahedral element and six truss elements. On each edge of the tetrahedron one truss element is attached which models the force-stretch behaviour of a bundle of polymer chains. Connecting this elastic behaviour of rubber-like material with the thermal one, the proposed method provides the possibility to observe how changes at the microscopic level influence the macroscopic material behaviour also under varying thermal conditions.The main focus of this work is the influence of both, the material constants and heat transfer boundary conditions on the response of shape memory polymers. To conclude we illustrate different examples of application.

Numerical simulation of the material behavior of pre-textured poly-crystalline shape-memory alloys. **Rainer Fechte-Heinen** (Ruhr-Universität Bochum, Germany), Klaus Hackl (Ruhr-Universität Bochum, Germany) GA/CT1959/006

We present a micromechanical model for polycrystalline shape-memory alloys. The main focus of our model is the orientation distribution of the austenitic and martensitic variants. We assume the material to consist of a large but finite number of randomly oriented crystallites in which the material is able to transform inbetween the high- and low-temperature-phase. The material behavior then originates from the accommodation of the orientation distribution of all variants in order to minimize the free energy density. By this ansatz, the internal reorientation of martensite can be predicted. Hysteresis effects are included via the hypothesis that changes in the orientation distribution are connected with energy dissipation by a function of first order. The model is capable of reproducing all essential effects in the material behavior of shape memory alloys such as pseudoelasticity and pseudoplasticity as well as the influence of pre-texture caused by the production process.

Experimental as well as numerical validation based on the works of Smyshlyaev & Willis are shown.

GA/CTS4455/06: Elastomers: testing, modelling and simulation.

Organiser: Rolf Mahnken (Universität Paderborn, Germany)
Co-organiser: Alexander Lion (Universität der Bundeswehr, Germany)

Zu den Auswirkungen von Selbstorganisationsprozessen auf das makroskopische mechanische Verhalten hochmolekularer Werkstoffe. **Jörn Ihlemann** (Deutsches Institut für Kautschuktechnologie, Germany) GA/CT3008/006

Die hochmolekularen Werkstoffe unterteilen sich gemäß ihrer mechanischen Eigenschaften grob in Duromere, Thermoplaste und Elastomere. Die Duromere sind räumlich eng vernetzt, zeigen ein weitgehend elastisches Verhalten und eine vergleichsweise geringe Verformbarkeit. Hingegen ist das mechanische Verhalten der Thermoplaste bei größeren Verformungen durch das plastische Abgleiten der nicht vernetzten Makromoleküle charakterisiert. Die technischen Elastomere zeigen eine Kombination großer, weitgehend reversibler Deformationen mit ausgeprägten, inelastischen Effekten und belastungsinduzierten Änderungen des stark nichtlinearen Materialverhaltens. Nach wie vor werden Ansätze zur physikalischen Erklärung dieser Eigenschaftskombination anhand des molekularen Aufbaus bezüglich ihrer Widerspruchsfreiheit zu physikalisch-chemischen und phänomenologischen Befunden diskutiert.

Ein großes Erklärungspotential zeigt die Theorie sich selbst organisierender Bindungsmuster (SOLP = Self-Organizing Linkage Patterns). Diese Theorie basiert auf der Annahme, daß sich während eines Belastungsvorgangs die Verteilungen der zwischenmolekularen, physikalischen Bindungen und ihrer jeweiligen Belastungen infolge massiver Auf- und Abbauraten zu einem im Verhältnis zu den ursprünglichen Unregelmäßigkeiten der molekularen Struktur großräumigen Muster prozeßspezifischer Inhomogenitäten aus verstärkten und entfestigten Bereichen organisieren. Der sich mit dem Muster entwickelnden Verschaltungscharakteristik der Bindungen innerhalb des molekularen Netzwerks wird eine wesentliche Bedeutung bezüglich des momentanen makroskopischen mechanischen Verhaltens unterstellt.

Zur Uberprüfung der Theorie und zur näheren Erforschung dieser Vorgänge dient ein Sondierungsprogramm, dessen Resultate die Existenz der Selbstorganisationsprozesse und deren unmittelbaren Zusammenhang mit dem mechanischen Verhalten der Gummimaterialien bestätigen. Durch aufwendige Abstraktionsmaßnahmen und speziell angepaßte numerische Algorithmen gelingen mit diesem Sondierungsprogramm im Rahmen moderater Computerkapazitäten Simulationen relevanter Prozesse, wobei wesentliche Effekte des mechanischen Verhaltens von Gummi reproduziert werden.

Experimental investigations on the mechanical behavior of filled rubber. **Michael Dämgen** (Medizinische Hochschule Hannover, Germany), Udo Nackenhorst (Leibniz Universität Hannover, Germany) GA/CT2108/006

The mechanical properties of technical rubber are roughly described by the non-linear elastic behavior but incompressible behavior with extremely high fracture tension, hysteretic behavior under cyclic conditions, stiffening under dynamic loading and damage due to overloading. This behavior is explained from the microstructure of elastomers and influenced by the basic polymer system, the treatment for networking and filler reinforcement. An amount of models exist to explain this behavior, but a suitable data-basis for model validation is missing. Therefore, in this contribution experimental studies on the mechanical behavior of well defined rubber systems will be presented. By uniaxial tension and compression tests the rubber-mixtures are compared regarding their stress softening (Mullins effect), remaining plastic strain, hysteresis, etc. These results will also be compared with those obtained from shear-tests. Additional measurements have been performed with respect to the characterization of damage induced anisotropy, relaxation behavior and temperature dependency of both, initial mechanical properties and annealing behavior. Besides a critical review of different measurement techniques on the reliability, the capability of state of the art models implemented in commercial finite element programs will be discussed.

Amplitude-dependent phenomena of filler-reinforced rubber: experiments, modelling and simulation. **Philipp Höfer** (Universität der Bundeswehr München, Germany) GA/CT2648/006

It's a matter of common knowledge, that carbon black- or silica-loaded elastomers show a pronounced nonlinearity when excited with dynamic deformation amplitudes, namely the Payne-effect. While intact at low amplitudes, the filler network is destroyed with increasing strains leading to a decrease in the storage modulus and to a distinct maximum in the loss modulus at intermediate amplitudes. Furthermore, several experiments prove a very complex history-dependence; for example, a significant recovery-behaviour after an amplitude jump or the observed hole-burning effect.

In the present talk, a few experimental results of dynamical measurements on filler-loaded rubber are shown with importance attached to the complicated history dependence. In order to describe the depicted phenomena, a thermodynamic consistent model of nonlinear viscoelasticity is presented. The model is based on intrinsic time scales which are driven among others by the current state of the filler network. In contrast to models in the frequency domain, the present formulation can be easily implemented into Finite-Elements and solved for arbitrary loading processes. Corresponding numerical results of the presented model are shown and compared with given experimental results.

On phenomenological and micro-mechanical models in finite elasticity and viscoelasticity for rubber-like materials. **Mokarram Hossain** (TU Kaiserslautern, Germany), Paul Steinmann (TU Kaiserslautern, Germany), Ralf Denzer (TU Kaiserlsautern, Germany) GA/CT2204/006

Nowadays, polymeric materials have many commercial and engineering applications. Some polymers not only show elastic behaviour but also complex time-dependent behaviour when subjected to a history of stress or strain. There are several phenomenological based models and micro-mechanically motivated network models for elastic and viscoelastic polymeric materials which have been proposed in the literature. The 8-chain, 3-chain models (elastic), full network models (elastic), micro-macro unit sphere (21-chain) models are well-known models which can be used for moderate to large elastic and viscoelastic deformations of polymeric materials. The Ogden model is one of the classical phenomenological models for elastic and viscoelastic polymeric materials.

The aim of the research work is to compare various phenomenological and micro-mechanical models for elastic and viscoelastic processes at large deformation.

Representation of static and dynamic elastomer behaviour and industrial applications. **Herbert Baaser** (Freudenberg AG, Germany) GA/CT1246/006

The aim of the talk is the description of a phenomenological material model incorporating the static and dynamic behaviour of elastomers for industrial applications such as seals and dampers. These highly nonlinear effects are connected with the names of MULLINS and PAYNE, respectively.

In that sense, we identify stress softening (MULLINS) and permanent deformation as inelasticity, and describe additionally the occurence of viscoelasticity (PAYNE) in parallel, which is typically known for elastomers to decrease the dynamic stiffness with increasing the strain amplitude.

These individual effects are covered separately in the constitutive law. This permits a largely modular design of the material description on the basis of user interfaces in commercial FE programs and a much easier parameter adjustment. On the as-

sumption of a multiplicative decomposition of the deformation gradient into a hyperelastic and an inelastic part, the modeling of metal materials within the scope of finite deformations has been established itself a considerable time ago. This concept is now adequately transferred to the considered material class and expanded accordingly.

In addition, the hyperelastic part of the material answer is defined on the basis of any freely chosen function of the strain energy (density), while the modeling of the inelastic parts is based on the formulation of a non-linear, isotropic hardening. The aforementioned description of stress softening in the hyperelastic part is additionally controlled by means of the first invariant of the elastic deformation. The branch of time domain viscoelasticity is realized by the use of a hereditary integral formulation and the help of PRONY series, where a well-defined parameter calibration is focused especially in that part of the presentation.

GA/CTS4452/06: Sintering, extrusion and plasticity.

Organiser: Marina Shitikova (Voronezh State University, Russian Federation)
Co-organiser: Alexander Lion (Universität der Bundeswehr, Germany)
Co-organiser: Rolf Mahnken (Universität Paderborn, Germany)

Simulating solid-state sintering and compaction of metal powder in the finite-strain regime. **Jan Frischkorn** (TU Braunschweig, Germany), Stefanie Reese (TU Braunschweig, Germany) GA/CT2281/006

Large ring-shaped workpieces manufactured by radial-axial ring rolling which are powder-metallurgically covered with wear resistant outer layers using the HIP-technology can be found in many industrial applications (e.g. mills for crushing mineral goods, bearing rings). The HIP-process limits the maximum possible ring diameter and is very expensive, too. A remedy to this problem is expected from integrating the sintering and compaction of the metal powder into the ring rolling process. For this purpose, a material model has been developed which is able to describe solid state sintering as well as compaction under high temperature where sintering effects are still active. The continuum mechanically-based model (derived on the basis of [1]) is formulated in the large strain regime to cover geometrical nonlinearities. Visco-plastic behaviour is described in form of an overstress function of the Perzyna type. Assuming an associative flow rule, the evolution equations of the internal variables can be derived from a pressure sensitive convex yield function. Furthermore, exploiting the Clausius-Duhem inequality guarantees thermodynamic consistency of the model. The use of an exponential mapping integration scheme ensures that the plastic compression described by the model is realistically simulated.
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Modeling and computation of metal powder compaction processes. **Stefan Hartmann** (Universität Kassel, Germany) GA/CT2256/006

Compaction processes of metal powder indicate the application of a finite strain plasticity model for very large volumetric compression behaviour to represent the experimental observations. In this lecture a new constitutive model based on a convex and unique single surface model using a logarithmic interpolation concept of two simpler yield functions is adapted to experimental data of die compaction experiments. The yield function is controlled by internal variables so that the convexity condition of the yield function and the thermo-mechanical consistency in the sense of the Clausius-Duhem inequality is satisfied during all possible compaction processes. The constitutive model is based on the multiplicative decomposition of the deformation gradient into an elastic and a plastic part, a hyperelasticity relation of Simo&Pister type using stress and strain measures relative to the plastic intermediate configuration and an associative flow-rule. This constitutive model is implemented into a time-adaptive finite element program using high-order diagonally implicit Runge-Kutta methods in combination with the Multilevel-Newton algorithm which are applied onto the DAE-system resulting from the vertical line method in the context of finite elements. This concept preserves the structure of currently applied implicit finite element programs. A known order reduction phenomenon and the influence of a Perzyna-type regularization will be studied. In this respect it becomes apparent that a Newton-Raphson method on Gauss-point level for computing the internal variables will fail in most situations. Accordingly, other solution procedures must be investigated. Here, a constrained line-search and an arc-length approach are studied showing that the line-search approach shows the most efficient choice.

Modeling and simulation of extrusion of aluminum alloys. **Tobias Kayser** (Universität Dortmund, Germany), Christian Hortig (Universität Dortmund, Germany), Farhad Parvizian (Universität Dortmund, Germany), Bob Svendsen (Universität Dortmund, Germany) GA/CT2287/006

The purpose of this work is the modeling and simulation of the material behavior of alumminum alloys during extrusion processes. In particular, attention is here focused on Al-Mg-Si alloys of the 6000 series, which are characterized by providing a maximum of ductility and Al-Zn-Mg alloys of the 7000 series, which show better hardness properties but reduced ductility. During extrusion the material behavior is governed by the process of dynamic recovery, whereas static re-crystallization is the dominating process during cooling. In both cases the current material model is based on the role of energy stored in the material during deformation as the driving force for microstructural development. Information about the developing microstructure (e.g., texture, dislocation structures, etc.) and the influence of process conditions such as extrusion rate and temperance affect on it are provided by experimental results. State quantities like dislocation density, average grain size and grain orientation are described by using the concept of internal variables. Constitutive equations for these quantities are formulated in a thermodynamically-consistent fashion as part of a thermo-elastic, visco-plastic model with heat conduction. Applications to the case of extrusion with cooling will be presented.

Flow of viscoplastic material through converging channels. **Sergey Aleksandrov** (Institute for Problems in Mechanics RAS, Russian Federation), Elena Lyamina (Institute for Problems in Mechanics RAS, Russian Federation), Gennady Mishuris (Rzeszow University of Technology, Poland) GA/CT443/006

Flow through converging channels is one of the classical problems in plasticity theory. The first solutions of this kind for both wedge-shaped and axisymmetric channels have been obtained for rigid perfectly/plastic material. Though subsequent generalizations of these solutions on other material models have been proposed, it is easy to verify by inspection that most of these generalizations fail in the case of the maximum friction law (this law postulates that the friction stress is equal to the local shear yield stress). This results from the fact that the qualitative asymptotic behaviour of solutions in the vicinity of maximum friction surfaces strongly depends on the constitutive law chosen. In particular, in the case of viscoplasticity none of available generalizations reduces to the classical solutions, though the viscoplastic model reduces to the model of classical rigid plasticity at certain set of parameters. It is therefore of interest to propose such a viscoplastic law that leads to a solution which does reduce to the classical one. In this way it is possible to construct a unified theory of plasticity which would cover a wide range of temperatures and strain rates with a continuous (in certain sense) transition of solutions from low temperatures and strain rates to high temperatures and strain rates. In the present paper a viscoplastic model with a saturation stress is adopted to find the solution for flow through wedge-shaped and axisymmetric channels. It is shown that the asymptotic behaviour of the solution in the vicinity of the maximum friction surface depends on the parameters of the model but there is a set of parameters at which the viscoplastic solution shows the same features as the classical solution.

The multiple intermediate configuration approach and its influence on DIRK/MLNA finite-element procedures. **Karsten Quint** (Universität Kassel, Germany), Stefan Hartmann (Universität Kassel, Germany) GA/CT2340/006

According to the proposals of Lion [1] and Tsakmakis/Willuweit [2] kinematic hardening can be modelled using an additional multiplicative decomposition of the plastic part of the deformation gradient in the multiplicative decomposition approach. In this context, two flow rules control the evolution of the intermediate configurations, which are formulated on the basis of the von Mises yield function in the Mandel stress space.

Both flow rules describe the *plastic incompressibility*. The application of Runge–Kutta like integration procedures can not guarantee the incompressibility condition. Accordingly, projection methods in the sense of geometry preserving method have to be applied.

In this lecture, stiffly accurate diagonally implicit Runge–Kutta methods (DIRK) in combination with the Multilevel-Newton algorithm (MLNA) are extended by a projection step so that plastic incompressibility is satisfied. Numerical studies are performed to investigate the achievable order of high-order integration methods, the time-adaptive behaviour and the influence of the geometry-preserving algorithm to the stability, accuracy and efficiency of the method under consideration.

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On the influence of phase-transformations on the experimental determination of micromechanical model-parameters. **Thorsten Bartel** (Ruhr-Universität Bochum, Germany), Klaus Hackl (Ruhr-Universität Bochum, Germany) GA/CT2508/006

In the context of a micromechanical model for materials undergoing multivariant solid–solid phase transformations, which has been developed by the authors, the question arises in which way certain quantities can be determined sufficiently. At a first glance, the question may appear trivial because it's a well established strategy to fit model-parameters like those governing the width and the height of hysteresis loops by comparing numerical results to experimental data. Yet, we entertain some doubts concerning this matter and would like to discuss whether tests on specimens are able to provide significant results in the aforementioned context at all.

To verify this, we discretize a specimen by finite elements and simulate tension tests taking different boundary conditions into account. We compare the respective results to each other and to the outcome of a material-point computation performed with our micromechanical model, respectively.

07, Short Communications

GA/CTS4778/07: **Thermomechanics.**

Organiser: Stefan Diebels (Universität des Saarlandes, Germany)
Co-organiser: Marc Kamlah (Forschungszentrum Karlsruhe, Germany)
Co-organiser: Guenther Meschke (Ruhr-Universität Bochum, Germany)

Thermo-mechanics of martensitic phase transitions in shape-memory alloys: experiments, modeling, and numerical simulation.
Dirk Helm (Fraunhofer IWM Freiburg, Germany) GA/CT3137/007

As a result of martensitic phase transitions, shape memory alloys exhibit a thermomechanical behavior, which cannot be observed in other materials. Therefore, shape memory alloys enable exceptional products like stents, endoscopic devices for minimally invasive surgery, and eyeglass frames. In order to develop and improve such innovative products, the structural behavior must be simulated in the framework of thermomechanics on the basis of experimental investigations.

In the first part of the present contribution, the thermomechanical behavior of shape memory alloys is discussed. Thereafter, the identified material properties are modeled in the framework of continuum thermomechanics. The proposed model is based on a free energy function and evolution equations for internal variables. Thermomechanical consistency is ensured in the sense that the constitutive model satisfies the Clausius-Duhem inequality. Finally, the proposed constitutive theory is numerically treated in the context of the finite element method in order to simulate the behavior of structures made of shape memory materials.

Coupled CFD analysis of hot gas and coolant flow in effusion-cooled combustion chambers. **Jörg Riccius** (DLR Lampoldshausen, Germany), Andreas Gernoth (DLR Lampoldshausen, Germany), Oskar Haidn (DLR Lampoldshausen, Germany) GA/CT3672/007

In order to increase the efficiency of currently available $10\,\mathrm{MPa}$ combustion chambers, hot gas pressures of up to $25\,\mathrm{MPa}$ are desirable. As such high pressures lead to an increased heat transfer from the hot gas into the combustion chamber wall, alternative cooling methods to the conventional regenerative cooling are required. One of the most promising alternative cooling approach is effusion cooling. The advantages of effusion cooling are damage tolerance and a comparatively low weight.

Since a few years DLR works on the field of effusion technology [1,2,3]. In the current abstract / paper, underlying CFD analyses are shown. These CFD analyses are based of the following principles:

- 1-degree 3D model (quasi-2D rotatory symmetric);
- solution of the Navier–Stokes equations;
- coupled analysis of the hot gas and the coolant flow in the combustion chamber (multi species);
- compressible flow;
- real gas;
- SST turbulence model in the combustion chamber and in the combustion chamber wall;
- in the combustion chamber wall: distributed resistance according to Forchheimer.

In a first step, the Forchheimer parameters, which describe the distributed resistance, are determined by means of a least square fit of experimental results with conical test samples. The excellent coincidence between the experimental and the numerical results with the least square fitted parameters confirms the validity of the Forchheimer model.

Based on the least-square-fitted Forchheimer parameters of the conical test samples, a coupled CFD analysis of the hot gas flow in the combustion chamber and the coolant flow in the combustion chamber wall is performed. The detailed analysis of the combustion itself is avoided by defining the injector plate of the combustion chamber as an inlet of the by-product of the combustion (steam). A good comparison between the experimentally and the numerically obtained mass flow rates can be obtained by fitting the turbulence parameters in the area of the porous medium.

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Dynamic and microstructural effects in a cylinder induced by the thermal pulse at its face. **Yaroslav Zhuk** (Timoshenko Institute, Kyiv, Ukraine), Olga Chervinko (Timoshenko Institute, Kyiv, Ukraine), Igor Senchenkov (Timoshenko Institute, Kyiv, Ukraine) GA/CT2223/007

Processes of generation and propagation of stress wave caused by the thermal impact at the face of long thin steel cylinder are investigated in the frame of coupled thermomechanics using thermodynamically consistent theory of inelastic material behavior. Dynamic problem statement is used. It is solved by FEM technique developed especially to treat the coupled thermomechanic behavior of inelastic material. Main properties of thermomechanical state in the vicinity of thermal pulse, stress wave propagation accompanied with temperature variation are studied as well as relationship between parameters of the thermal pulse and stress wave.

Microstructural transformations in a cylinder made of martensitic steel induced by the thermal pulse at its face are investigated as well. Material behavior is simulated by the same coupled thermo-viscoplastic model. The model is modified to take account for the microstructural transformations. To calculate the new phase generated under cooling of austenitic state the continious cooling transformation (CCT) diagrams are utilized. The change in microstructural state of martensitic component is accounting by the volume change as well as change of Bodner-Partom model parameters in appropriate way.

Evolutions of structural state and residual strain-stress state as a result of cooling are studied. The cooling regimes causing the formation of residual compressive stresses in the vicinity of the face are determined.

A mortar method for thermomechanically coupled problems. **Elke Berend** (Universität Hannover, Germany), Peter Wriggers (Universität Hannover, Germany), Udo Nackenhorst (Leibniz Universität Hannover, Germany) GA/CT2172/007

The demand for the development of numerical models for thermomechanically coupled contact problems receives impulses from various sectors of the industry. Regarding the foundry industry the final quality of casting products depends on the appearance of residual stresses, warping and size alterations. The numerical prediction of quality defects requires an application of more detailed constitutive material equations and the precise modelling of the cast/mould interaction during the solidification process. Within the latter the contact-dependend heat transfer between the metal and the mould plays a decisive role.

Due to the discrete nature of the constraint enforcement com-

monly used node-to-segment formulations for contact interaction show discontinuities in the transmission of contact pressure. Using the mortar method pointwise constraints across the internal interfaces are replaced by suitable weak continuity conditions which prevent the inconsistencies mentioned above. Within the mortar approach the contact surfaces are connected via Lagrange multipliers which are introduced on the boundaries of the contacting bodies. In this approach an interpolation of these multipliers with dual basis functions is proposed. Due to this choice a degree of freedom reduction is straightforward such that the Lagrange multipliers can be eliminated within a direct solution method. Hence the global system of equations only includes displacement degrees of freedom which leads to more robust algorithms when dealing with semi-solid metal.

Based on this development an extension of this approach to thermomechanically coupled problems is presented including heat conductance and radiation which depend on the contact pressure and the formation of local gaps, respectively.

Physical aspects of mathematical description of the Doppler's effect. **Józef Rafa** (WAT Military University of Technology, Poland), Gawinecki Jerzy Gawinecki (Military University of Technology, Warsaw, Poland) GA/CT1325/007

We present the Doppler effect as a solution to an wave equation concerning waves generated by a moving in space source of the wave that periodically changes itŠs signal in time. The solution has been reached by basing on the Cagniard - de HoopŠs method. The reached conclusion of the analysis proves that the Doppler effect presents the change in the frequency of the received signal as well as the change of itŠs phase. In conclusion these changes are inhomogeitic and anizotropic. This research has been successfully applied in telecommunication and in locating sources of radiation of electromagnetic waves.

GA/CTS4779/07: Ferroelectrics.

Organiser: Dirk Helm (Fraunhofer IWM Freiburg, Germany)
Co-organiser: Marc Kamlah (Forschungszentrum Karlsruhe, Germany)
Co-organiser: Guenther Meschke (Ruhr-Universität Bochum, Germany)

Micro-electromechanical concepts for modelling ferro- and piezoelectric materials. **Johannes Rödel** (German University in Cairo, Egypt) GA/CT4254/007

Ferro-electric ceramic materials usually show micro-structural features on different length scales. They are polycrystalline solids with crystallites of random crystallographic orientations. The crystallites are divided into ferroelectric domains of differently oriented spontaneous polarizations and associated strains. The domains are crystallographically correlated and form often hierarchical patterns where the grains consist of blocks or bands which in turn consist of a fine domain structure. These domain patterns can change by switching the local polarization and associated strain under sufficiently large applied fields or loads. This leads to a macroscopic behavior of the ceramic material, including non-linear electro-mechanical response and hysteresis, which is very different from local single crystal response.

The aim of micro-electromechanical constitutive models is to describe and to calculate the macroscopic electro-mechanical response of ferroelectric polycrystals on the basis of microscopic properties and simplified micro-structural descriptions of the material. From this point of view, micro-mechanics provides the classical approach to bridge scales within the framework of continuum mechanics.

The present work will demonstrate the usage of simple microstructural models, like laminates and matrix-inclusion-models, to build a complex hierarchical homogenization theory. Within this model, the non-linear behavior of ferroelectrics is a result of changes of the microstructure by moving domain walls and local switching of the ferroelectric polarizations under applied fields.

Simulation of micro-cracking in ferro-electric materials based on a cohesive-type approach. **Johannes Utzinger** (TU Kaiserslautern, Germany), Andreas Menzel (Universität Siegen, Germany), Paul Steinmann (TU Kaiserslautern, Germany) GA/CT1967/007

Ferroelectric materials exhibit a huge potential for engineering applications, ranging from electrical actuators (inverse piezoelectric effect) to sensor technology (direct piezoelectric effect). To give an example, lead zirconate titanate (PZT) is a typical perovskite ion crystal possessing ferroelectric properties. In this contribution, we are particularly interested in the modelling of microcracking effects in ferroelectric materials.

In view of Finite-Element-based simulations, the geometry of a natural grain structure, as observed on the so-called micro-level, is represented by an appropriate mesh. While the response on the grains themselves is approximated by coupled continuum elements, grain boundaries are numerically incorporated via so-called cohesive-type elements. For the sake of simplicity, switching effects in the bulk material will be neglected. The behaviour of the grain boundaries is modelled by means of cohesive-type laws. Identifying grain boundaries as potential failure zones leading to microcracking, cohesive-type elements consequently offer a great potential for numerical simulations. As an advantage, they do not result in bad-conditioned systems of equations as compared with the application of standard continuum elements to localised deformations. Finally, representative constitutive relations for both the bulk material and the grain boundaries, enable two-dimensional studies of benchmark boundary value problems.

A fully-coupled nonlinear thermoelectromechanical model for piezolaminated smart structures. **Sven Lentzen** (RWTH Aachen, Germany), Ruediger Schmidt (RWTH Aachen, Germany) GA/CT1974/007

In present engineering applications piezoelectric materials gain increasing importance in the development of smart structures; e.g., for shape and vibration control problems. Such structures exhibit a three-way coupling effect between the mechanical, electrical and thermal quantities. In the majority of papers available in literature this coupling is taken into account only in the constitutive equations. It is however well known that truly coupled analysis should also be based on the interaction of the mechanical, thermal and electrostatic quantities in the field equations. Only in this way many physical effects can be taken into account; e.g., the strain rate dependant change of temperature due to mechanical loading. Furthermore most of the analyses conducted in this area are performed in the linear range of deformations assuming small strains, rotations and temperature changes. However smart technology is generally applied to thin walled structures and in many cases reported in literature are much large than the thickness, which results into geometrically nonlinear behaviour; like e.g., the occurrence of stress stiffening which greatly affects the prediction of sensor voltage outputs.

The present paper deals with the fully coupled thermoelectromechanical analysis of piezolaminated structures in the sense mentioned above, uncluding the geometrical and thermal nonlinear effects. A thermodynamically consistant contin-

uum mechanics based framework is developed, which includes the conservation of mass, linear and angular momentum and the conservation of energy. The second principle of thermodynamics is used to derive the restrictions for the constitutive equations using Coleman–Noll analysis approach. The resulting set of equations is more general and valid for a wider class of problems than most models published in literature. For the sake of general applicability all equations are derived with respect to convective curvilinear coordinates.

On the piezoelectric shear effect in ultrasonic motors. **Martin Schönecker** (TU Darmstadt, Germany), Ana Conrado (TU Darmstadt, Germany) GA/CT2352/007

A new actuator concept for piezoelectric ultrasonic motors (USM) using the d_{15} effect is considered. Whereas the piezoelectric d_{33} and d_{13} effects are normally used in commercial motors, there exist hardly any USM based on shear actuation. Prototypes existing in the literature are described briefly.

After a short literature review, the paper introduces a new concept for actuation using the d_{15} effect. It is described analytically by deriving and solving the equations of motion for a shear actuator with voltage excitation. An optimization is performed with respect to the dynamic piezoelectric coupling factor. Suitable superposition leads to ultrasonic traveling waves capable of driving a rotor. The feasibility of the concept is demonstrated by a first prototype motor produced in our lab in Darmstadt.

An incremental variational formulation for the coupled electro-mechanical response of piezo-ceramics. **Daniele Rosato** (Universität Stuttgart, Germany) GA/CT4065/007

The paper presents continuous and discrete variational formulations for the treatment of the non-linear response of piezoceramics under multiaxial electromechanical loading. The point of departure is a general internal variable formulation that determines the hysteretic response of the material as a generalized standard medium in terms of an energy storage and a dissipation function. Consistent with this type of standard dissipative continua, we develop an incremental variational formulation of the coupled electromechanical boundary value problem. We specify the variational formulation for a setting based on a of smooth switching-surface which governs the hysteretic response. An important aspect is the numerical implementation of the coupled problem. The discretization of the two-field problem appears, as a consequence of the proposed incremental variational principle, in a symmetric format. The performance of the proposed methods is demonstrated by means of a spectrum of benchmark problems.

GA/CTS4776/07: Magnetomechanics.

Organiser: Marc Kamlah (Forschungszentrum Karlsruhe, Germany)
Co-organiser: Guenther Meschke (Ruhr-Universität Bochum, Germany)

Modeling of coupling phenomena in multifunctional materials. **Bjoern Kiefer** (Universität Stuttgart, Germany) GA/CT1775/007

The recent emergence of new active and multifunctional materials, such as ferroelectrics (piezoceramics) and magnetic shape memory alloys (MSMAs), has posed new challenges for constitutive modeling. The complexity of the constitutive response that such materials exhibit is due to its typically nonlinear and hysteretic nature as well as the intrinsic coupling of thermal, mechanical, electric and magnetic effects.

The presented work addresses three different aspects of the modeling process, the formulation of phenomenological constitutive models for MSMAs and ferroelectrics, which are based on an extended thermodynamic framework and utilize internal state variables to capture hysteretic effects and loading history dependence, the numerical implementation of such constitutive models into a finite element environment and the numerical analysis of coupled boundary value problems.

Magnetostrictive actuation of a smart beam with hysteretic material behaviour. **Heiko Bossong** (RWTH Aachen, Germany), Ruediger Schmidt (RWTH Aachen, Germany) GA/CT1715/007

Magnetostrictive materials can be used as actuators in smart structures technology. The relation between induced strain and the applied magnetic field is nonlinear and shows hysteretic behaviour. Thus the magnetomechanical coupling coefficient is not constant and should be defined as a function of strain or magnetic field in computations.

In this study the hysteresis of a mechanically unconstrained actuator is determined using the Michelson interferometry. The hysteretic behaviour is modelled phenomenologically by a Preisach model. Using these experimental data for the modelling of an active structure with embedded magnetostrictive actuators, the actual coupling coefficient can be determined utilising the Preisach model. With this procedure the actuation strain of an embedded actuator, including the physical nonlinearities, can be calculated using the material characteristics obtained with an unconstrained actuator. For the determination of the actual coupling coefficient a strain and field dependent approach is used.

For an experimental validation of the method outlined above, a magnetostrictive actuator is characterised experimentally and then applied to a cantilever aluminium beam. Then, the tip displacement of the actuated beam is measured with a laser triangulation sensor.

Geometrically nonlinear finite-shell elements with magnetostrictive layers. **Ruediger Schmidt** (RWTH Aachen, Germany), Sven Lentzen (RWTH Aachen, Germany) GA/CT1988/007

The area of smart structural control has raised the interest of many researchers in the field of mechanical, electrical, material and control engineering. A relatively small number of material types have proven suitable to be applied as sensors and/or actuators; e.g., piezoelectric and magnetostrictive materials and shape memory alloys. A wide variety of literature can be found dealing with the modelling of piezoelectric materials. Considerably less publications can be found about the latter two materials, especially when geometrical nonlinearity is concerned.

In this paper a geometrically nonlinear composite shell element with integrated magnetostrictive layers is presented. Three translational and two rotational nodal degrees of freedom are used for the first-order transverse shear approximation. The finite element is used in order to investigate shape and stability control problems of structures with magnetostrictive actuator layers in the range of large deformations. The numerical approximations to this static problem are obtained using the total Lagrangian formulation for the moderate rotation shell theory. The aforementioned finite element is used to numerically investigate the actuation behaviour of the integrated magnetostrictive layers. Since the magnetic field is prescribed, the

coupled magnetoelastic problem turns into a decoupled problem. In the final paper a few examples of thin-walled plates and shells with integrated magnetostrictive layers will be presented.

3D multifield modelling of electromagnetic metal forming processes. **Jaan Unger** (Universität Dortmund, Germany), Bob Svendsen (Universität Dortmund, Germany) GA/CT2290/007

Electromagnetic metal forming is a contact-free high-speed forming process in which strain rates of more than 10^3 s^{-1} are achieved. The deformation of the workpiece is driven by a material body force, the Lorentz force, that results from the interaction of a pulsed magnetic field with eddy currents induced in the workpiece by the magnetic field itself.

The purpose of this work is to present a fully-coupled 3D simulation of the process. For the mechanical structure a thermoelastic, viscoplastic, electromagnetic material model is relevant, which is incorporated in a large-deformation dynamic formulation. The evolution of the electromagnetic fields is governed by Maxwell s equations under quasistatic conditions. Their numerical solution in 3D requires particular arrangements due to a reduced regularity at material interfaces. Hence, Nédélec elements are employed. Coupling between the thermomechanical and electromagnetic subsystems takes the form of the Lorentz force, the electromotive intensity, and the current geometry of the workpiece in the electromagnetic domain. A staggered scheme based on a Lagrangian mesh for the workpiece and an ALE formulation for the electromagnetic field is utilized to solve the coupled system, guaranteeing the efficiency and accuracy of the data transfer between the two boundary-matching meshes. This mesh adoption allows for a special data mapping of the strongly decaying Lorentz forces in the thickness direction of the workpiece. In contrast to other simulation examples where continuum elements are applied this data mapping approach allows for the use of highly efficient solid shell elements.

Problem of magneto-elasticity for a solid with the spherical cavity. **Olga Dashko** (Timoshenko Institute, Kyiv, Ukraine) GA/CT934/007

The solution of a static problem of magnetoelastisity for a soft ferromagnetic elastic solid with the spherical cavity is obtained on the base of the linear theory of Brown, Pao and Yeh. It is assumed that the solid has a multi-domain structure, so the hysteretic loss and remanent magnetization are neglected. The solid is affected by a magnetic field which is uniform at infinity and determined by the magnetic induction vector. The cavity causes some distortion of the field distribution near the interface. So the field induces magnetic moments and produces stresses and deformations in the body. The problem is solved for an unperturbed strain state. An approach is discussed to find the perturbed values on the base of the solution obtained. The Fourier variable separation method is used. The stresses are presented via harmonic functions. As a result magnetoelastic stresses are obtained in the closed form. Their distribution in the body is studied and some results of numerical calculations are shown.

GA/CTS4782/07: Numerical mechanics.

Organiser: Detlef Kuhl (Ruhr-Universität Bochum, Germany)
Co-organiser: Marc Kamlah (Forschungszentrum Karlsruhe, Germany)
Co-organiser: Guenther Meschke (Ruhr-Universität Bochum, Germany)

Coupled problems in biomechanics and medical technology. **Markus Böl** (TU Braunschweig, Germany), Stefanie Reese (TU Braunschweig, Germany), Daniel Christ (TU Braunschweig, Germany) GA/CT3472/007

The contribution focuses on multi-field problems in the context of applications of biomechanics and/or medical technology. The first example concerns the finite element modelling of sceletal muscles the activation of which can be mathematically described as follows. Based on a distribution function we determine the action potential in dependence of space and time. This action potential leads to an increase of the Calcium concentration. The latter two steps require the solution of two differential equations. It is further noted that the Calcium diffusion is dealt with by introducing another degree-of-freedom at each finite element node. When the Calcium concen-tration reaches a certain limit the muscle contraction begins (single twitch). Finally a summation over the motor units is carried out which gives us finally the mechanical response of a single muscle fibre. The behaviour of the total muscle is computed as discussed in [1]. In medical technology, e.g. to manufacture intracranial stents, the special properties of shape memory alloys and polymers are used frequently. In both cases the structure is able to recover its original state. In the context of shape memory alloys this phenomenon is called pseudo-elasticity or shape memory effect, depending on whether the behaviour is stress- or temperature-induced. Much less well-known is the fact that polymers may also exhibit a so-called shape memory effect which is, however, due to the significant change of material properties in the glass transition range. To describe this phase transition another variable is introduced which can be either (1) directly linked to the temperature, (2) have the status of an internal variable or (3) a field variable. The different possibilities are discussed. Due to the shape memory effect the deformation obtained up to a certain point is "frozen" when the temperature reaches the glass transition range from the above. Heating up the structure beyond the glass transition temperature the orginal state is recovered. This behaviour is exploited e.g. in the context of stents or medical threads. The talk closes with several numerical applications where also aspects as solution methods and coupling strategies are discussed.

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Coupled time-domain analysis with boundary and finite elements. **Thomas Rüberg** (TU Graz, Austria), Martin Schanz (TU Graz, Austria) GA/CT2358/007

The numerical analysis of dynamic soil-structure interaction is impeded by the soil half-space surrounding the region of interest. Standard finite element methods (FEM) truncate the mesh and thereby produce artificial wave reflections at the non-physical boundaries. The boundary element method (BEM) does not suffer from this deficiency by an implicit fulfilment of the radiation condition. Nevertheless, it does not provide the robustness and reliability as the FEM when applied to large deformations, plastifications or other non-linear effects.

Therefore, the application of both methods by certain coupling strategies is a well-established means to make use of the respective advantages of the method. So far, iterative coupling

strategies usually depend on some empirically chosen relaxation parameters which are problem-dependent. Therefore, a direct coupling approach is more robust.

A drawback in most coupling strategies is the strong fulfilment of the interface conditions which requires matching interface discretizations. This restriction is too severe when dealing with large substructures, whose meshes are commonly generated independently, and does not obey the different stability criteria for different numerical methods, especially in dynamic analyses.

In this work, an algorithm is presented which allows for different numerical methods (e.g., FEM and BEM) in the sub-domains and is not restricted to conforming interface discretizations. Whereas this idea, similar to the *Mortar* methods, is well-established for the analysis of static problems, it will here be transfered to time-domain problems. This is basically done by formulating so-called Dirichlet-to-Neumann maps in a discrete setting, which can be given by either method, and combining them with Lagrange multpliers in a weak form. Additionally, an efficient solution procedure for the resulting saddle point problems will be proposed for applications to the acoustic wave equation and elastodynamic problems.

Higher-order energy consistent-time integrators for nonlinear thermo-viscoelastodynamics. **Michael Gross** (Universität Siegen, Germany), Peter Betsch (Universität Siegen, Germany) GA/CT1660/007

Although the temporal finite element method is well-known since many years, for the temporal discretisation the finite difference method is still preferred. An advantage of the temporal finite element method is that higher-order accurate time integrators can be constructed easily. A further important advantage is the inherent energy consistency if applied to the equations of motion of dynamical systems [1]. The temporal finite element method is therefore used to construct higher-order energy-momentum conserving time integrators [2]. These time integrators turned out to be well suited for computing motions in nonlinear elastodynamics. Considering finite motions of a flexible solid body with internal dissipation, an energy consistent time integration is also of great advantage (see the references [3,4,5]).

In this presentation, we show that an energy consistent time discretisation is also advantageous for dynamics with dissipation arising from conduction of heat together with internal viscous dissipation. We start by deriving energy consistent fully weak evolution equations for all state variables (configuration, linear momentum, entropy and viscous internal variable) directly from the total energy of the system. The energy consistency is preserved by using a new enhanced hybrid Galerkin (ehG) method. The obtained numerical schemes satisfy the energy balance exactly independent of their accuracy order and the used time step size. This guarantees numerical stability.

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Effective parallelized co-simulation of mechatronic systems with subsystems integrated by different methods. **Markus Friedrich** (TU München, Germany), Heinz Ulbrich (TU München, Germany) GA/CT2231/007

This paper describes a method for coupling dynamic subsystems, which are originally independent, by Co-Simulation. This gives the possibility to simulate systems consisting of various domains and simulators. Each subsystem can use a totally different integration method (e.g. ODE, DAE or Time-Stepping) and can even be closed source, because the Co-Simulation is only based on input and output numerical data at the macro time steps. In case of mechanical subsystems the coupling is done on kinetic level by force laws. By introducing a modular master-slave concept it is also possible to parallelize the computational cost of each subsystem, when using a multiprocessor/-core system or even a cluster. The scalability of this parallelization is mainly affected by the overhead of the subsystem communication. On the site of information engineering this problem is to be concerned with PVM, MPI or shared memory techniques for effective and fast inter process communication and synchronization. On mathematically side this is concerned with a higher order discretization of the coupling force to increase the macro step size which also leads to better scalability. Lastly this method is applied on an industrial example in form of a Co-Simulation between a timing chain drive and a valve train.

GA/CTS4775/07: Porous media, I.

Organiser: Guenther Meschke (Ruhr-Universität Bochum, Germany)
Co-organiser: Marc Kamlah (Forschungszentrum Karlsruhe, Germany)

On coupled problems in geomechanics. **Wolfgang Ehlers** (Universität Stuttgart, Germany) GA/CT4081/007

Geomechanical problems are generally based on the category of granular, cohesive-frictional materials with a fluid pore content. At the macroscopic scale of continuum mechanics, these materials can be successfully described on the basis of the well-founded Theory of Porous Media (TPM) [1].

The present contribution touches fundamental problems of coupled media by investigating the interacting behaviour of an elasto-viscoplastic porous solid skeleton, the soil, and two pore fluids, water and air. Furthermore, electro-chemical reactions are considered in order to include the swelling behaviour of active soil. In conclusion, this leads to a system of strongly coupled partial differential equations (PDE) that can be solved by use of the finite eelment method (FEM). In particular, the presentation includes fluid-flow situations in the fully or the partially saturated range, swelling phenomena of active clay as well as localization phenomena [3,4] as a result of fluid flow or heavy rainfall events. The computations are carried out by use of the single-processor FE tool PANDAS[1] and, in case of large 3-d problems, by coupling PANDAS with the multi-processor solver M++.

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A three-phase FE-model for the simulation of partially saturated soils. **Felix Nagel** (Ruhr-Universität Bochum, Germany), Guenther Meschke (Ruhr-Universität Bochum, Germany) GA/CT4069/007

While for many computational analysis in geotechnics use of a two-phase model is sufficient, separate consideration of all three phases is mandatory for numerical simulations of partially saturated soils subjected to compressed air. This is a common technique frequently applied for temporary ground support in tunnelling. For the numerical simulation of tunnelling using compressed air, a multiphase model for soft soils is developed, in which the individual constituents of the soil - the matrix, the fluid and the gaseous phase - and their interactions are considered.The three phase model is formulated within the framework of the mixture theory, based upon balance equations (momentum balance of the mixture, mass balance of the fluid and gaseous phase) and constitutive relations for the soil skeleton, the pressure-density relation of the gaseous phase, the pressure-suction relation and the pressure-seepage flow relation. Water is modelled as an incompressible and air as a compressible phase. The three phase soil model is implemented within an object-oriented FE-code developed for numerical simulations of shield tunnelling. Selected results from 3D simulations of a repair intervention in shield tunnelling with face support accomplished by means of compressed air will be presented.

A numerical model for partially saturated soils. **Günter Hofstetter** (Universität Innsbruck, Austria), Roman Kohler (Universität Innsbruck, Austria) GA/CT3767/007

The contribution deals with the numerical simulation of the behavior of partially saturated soils within the framework of a coupled three-phase model. In contrast to constitutive models for water saturated soils, which are formulated in terms of a single effective stress variable, some fundamental features of partially saturated soils can only be taken into account using two stress state variables. In the present case the employed stress state variables are (i) the Bishop stress tensor with the Bishop parameter being equal to the degree of water saturation and (ii) suction.

Using these two stress state variables, an elastic-plastic cap model for soils with a shear failure surface and a strain hardening cap is extended in order to represent the behavior of partially saturated soils by taking into account the dependence of the evolution of the shear failure surface and of the hardening of the cap on suction.

The capability of the developed constitutive model is demonstrated by the numerical simulation of a series of suction controlled tests, conducted by Macari et al., involving hydrostatic compression tests, triaxial compression tests, conventional triaxial compression tests, triaxial extension tests and simple shear tests. All these tests were conducted at three different values of suction.

Finally, the three-phase FE-formulation with the constitutive model for partially saturated soils is applied to the numerical simulation of a laboratory test, conducted by Klubertanz, in which a sand column is subjected to a few cycles of dewatering and subsequent watering.

Modeling wave propagation in porous media. **Holger Steeb** (Universität des Saarlandes, Germany) GA/CT2441/007

We discuss the acoustic phenomena of propagating waves within empty and fluid-saturated porous media. Linear acoustic models of porous materials were first introduced in the pioneering contributions of M. Biot (1956) and Y. Frenkel (1944). The famous Biot model of a biphasic porous material consisting of material compressible solid and fluid constituents is characterized by three propagating wave types: the shear wave, and, a fast and a slow compressional wave.

In the present contribution, we present an alternative modeling approach based on the thermodynamically consistent Theory of Porous Media. We show, that in the low frequency regime the dispersion relations of the so-called hybrid limit (bulk modulus of the *solid grains* $K^s \to 0$) are identical for both modeling approaches. Furthermore, several extensions towards more sophisticated models are presented. In addition to modeling purposes, we discuss the relating initial boundary value problems with respect to their numerical treatment in Galerkin finite elements and staggered finite difference methods.

Modeling of timing belt's construction. **Grzegorz Domek** (Kazimierz Wielki Univesity of Bydgoszcz, Poland) GA/CT3538/007

Mathematical description of materials used in belts production appeared to come very close to the real characteristics. Some software allow for introduction of real characteristics and in such conditions it is easier to relate to the real conditions in gears with timing belts. Experimental research confirm essentiality of timing pulley construction for cooperation with timing belt. New materials used in belt construction especially composites oblige us for further research of new belts constructions through experimental research.

GA/CTS4781/07: Porous media, II.

Organiser: Guenther Meschke (Ruhr-Universität Bochum, Germany)
Co-organiser: Detlef Kuhl (Ruhr-Universität Bochum, Germany)
Co-organiser: Marc Kamlah (Forschungszentrum Karlsruhe, Germany)

Modelling multiphase materials: Biot's theory vs. theory of porus media. **Stefan Diebels** (Universität des Saarlandes, Germany), Holger Steeb (Universität des Saarlandes, Germany), Zhiyun Chen (Universität des Saarlandes, Germany) GA/CT1684/007

The behaviour of multiphase materials like fluid-saturated soil, gas-filled foams or biological tissues can be described on a macroscopic scale either by Biot's theory (BT) or by the theory of porous media (TPM). It is shown that both approaches lead to a set of comparable equations which describe the same effects, e. g.which allow for the propagation of a second compressional wave (Biot wave). While Biot's theory is formulated in an intuitive way the theory of porous media is built upon a few axioms. Therefore, a non-linear formulation of the TPM is inherent. Several nonlinear but consistent extensions of the TPM are presented and their physical relevance is discussed. A robust numerical treatment of the resulting equations by space-time coupled Galerkin methods is presented.

Space-time FEM applied to wave propogation in porous media. **Zhiyun Chen** (Universität des Saarlandes, Germany), Holger Steeb (Universität des Saarlandes, Germany), Stefan Diebels (Universität des Saarlandes, Germany) GA/CT1883/007

In the present contribution, we formulate and apply a novel Hybrid Velocity Integration (HVI) scheme [2] to a biphasic mixture model describing the deformation behavior of fluid-saturated porous media. By integrating the displacement-velocity relation implicitly, the governing set of equations can be solved by the first-order Time-Discontinuous Galerkin method (DGT) c.f.[1]. The resulting equation system is solved sequentialy upon a coupled space-time finite element mesh. Inconsistent primary quantities over the time intervals are allowed. Furthermore, unlike the conventional DG penalty method, the continuity is enforced by a natural *upwind* flux. Besides, by adjusting the displacement-velocity integration scheme, the method can be easily identified with an implicit formulation, which stablized the solution immensely.

Numerical examples demonstrate the efficiency of the proposed method in comparison with standard discretization schemes based on the MOL. Furthermore, by applying the numerical solution technique to a so-called hybrid mixture model consisting of a material compressible pore-fluid and a materially incompressible solid constituent, we show, that the (highly attenuated) slow compressional wave (Biot's slow wave) can be calculated efficiently.

[1] Z. Chen, H. Steeb, S. Diebels.; A time-discontinuous Galerkin method for the dynamical analysis of porous media. Int. J. Numer. Anal. Meth. Geomech. 2006; **30**:1113–1134.

[2] Z. Chen, H. Steeb, S. Diebels; A new hybrid velocity integration method applied to elastic wave propagration. submitted to Int. J. Numer. Meth.,Eng.

A general modeling and numerical analysis framework for coupled processes. **Guenther Meschke** (Ruhr-Universität Bochum, Germany), Sandra Krimpmann (Ruhr-Universität Bochum, Germany), Detlef Kuhl (Ruhr-Universität Bochum, Germany) GA/CT4098/007

The present paper is concerned with a generalized procedure for the modeling and numerical analysis of multiphysics problems in computational structural and computational durability mechanics. The multiphysics model is constituted by generalized balance equations, constitutive laws which may include internal variables and, finally, the formulation of driving forces as function of the gradient of primary variables. As basis for the numerical solution of the fully coupled system of non-linear time dependent differential equations the weak form is formulated and linearized with respect to the primary variables. For the numerical analysis of the coupled system the semidiscretization technique is applied. In particular, a generalized multiphysics finite element with hierarchically generated shape functions is proposed. The time integration of non-linear first order semidiscrete initial value problems is performed by discontinuous and continuous GALERKIN schemes of arbitrary polynomial degree. Within this general modeling and simulation framework specific multifield problems can be implemented only on the GAUSS point level of the proposed general multiphysics element. The functionality of the present modeling and numerical analysis environment will be demonstrated by means of illustrative examples. The application to the life time prognosis of concrete structures subjected to mechanical and chemical attack will be discussed as a particular example in a separate paper [1].

[1] S. Krimpmann, D. Kuhl, G. Meschke, *Modeling and Numerical Analysis of Chemo-Mechanical Damage of Concrete within a General Multiphysics Framework*, GAMM 2007.

Modeling and numerical analysis of chemo-mechanical damage of concrete within a general multiphysics framework. **Sandra Krimpmann** (Ruhr-Universität Bochum, Germany), Detlef Kuhl (Ruhr-Universität Bochum, Germany), Guenther Meschke (Ruhr-Universität Bochum, Germany) GA/CT4094/007

The paper is concerned with a coupled chemo-mechanical damage model describing the interaction of highly non-linear dissolution and transport processes as well as mechanical damage in cementitious materials. For the purpose of reproducing the local chemical reaction and the additional diffusion exactly on the microlevel, a dissolution-diffusion model is developed within the framework of a general multiphysics model [1]. In particular, the ONSAGER & FUOSS model of electrolyte diffusion in chemically inert porous materials based on the theory of ionic clouds by DEBYE & HÜCKEL is presented. This electrolyte diffusion model is able to represent the electric charged mass transport and covers the ion-ion interaction. Furthermore, a reaction kinetics model for portlandite dissociation due to water attack $Ca(OH)_2 \rightleftharpoons Ca^{2+} + 2\ OH^-$ is investigated. This equation indicates the relevance of the amount of calcium ions within the pore space with regards to the state of chemical equilibrium. The ARRHENIUS equation provides the quantitative basis of the relationship between the activation energy and the rate at which the reaction of this dissolution process takes place. The material degradation due to chemical matrix dissolution and mechanical induced damage is captured by an isotropic scalar damage model with an equivalent strain damage criterion. As a representative example the numerical analysis of the model within a general framework [1] is used for the life time prognosis of a concrete beam subjected to mechanical and chemical attack.

[1] D. Kuhl, S. Krimpmann, G. Meschke, *A General Modeling and Numerical Analysis Framework for Coupled Processes*, GAMM 2007.

A numerical method to approximate the solutions of non-linear absorption–diffusion equations. **Alexandru Dumitrache** (ISMMA - Bucharest, Romania) GA/CT3135/007

In this paper, it is developed a numerical method in order to approximate the solutions of one-dimensional, non-linear absorption-diffusion equations. The method is tested for accuracy against a linear diffusion equation with a solution that can be written in closed form. Then various types of diffusion and absorption terms to determine which ones produce extinction in finite time are tested. Also the numerical solutions of the one-dimensional, non-linear absorption-diffusion equation and the diffusion-free equation are compared and one find that for the cases tested, the numerical absorption-diffusion solutions are always less than the numerical diffusion-free solutions. Furthermore, we find this is true for the cases tested when there is finite and infinite extinction time. We also look at the open problem where we have slow diffusion and weak absorption but, their combined effect is strong.

GA/CTS4777/07: Multiscale approach.

Organiser: Johannes Rödel (German University in Cairo, Egypt)
Co-organiser: Marc Kamlah (Forschungszentrum Karlsruhe, Germany)
Co-organiser: Guenther Meschke (Ruhr-Universität Bochum, Germany)

Atomistic simulations of the shape-memory effect in Lennard–Jones crystals. **Oliver Kastner** (Ruhr-Universität Bochum, Germany) GA/CT1830/007

We present 2D molecular dynamic simulations with an array of 32 small Lennard-Jones crystals. The individual crystals consist of nested lattices of two atom species. Distinct lattice structures can be identified, interpreted as austenite and (variants of) martensite. Temperature and/or load induced phase transitions between these configurations are observed in the simulations.

In previous work the thermal equation of state of one isolated crystal was investigated [1,2]. The crystal is small and it transforms uniformly between austenite and martensite. In the present contribution we investigate an array of such crystals, which are linked along an axis ("chain"). In this regard, the the individual crystals are interpreted as ideal lattice elements of a larger body. The chain is then investigated in numerical tensile tests under load and under displacement control for different temperatures.

The results show that –assuming simple Lennard-Jones potentials of interaction between atoms– the crystal chain allows for the simulation of the fascinating behavior of shape memory alloys, including pseudo-plasticity, pseudo-elasticity and the shape memory effect. The load/strain behavior of the chain assembly is determined by the collective load/strain response of the individual crystals according to temperature and loading conditions. Pseudo-plasticity appears as the result of martensitic de-twinning of the chain upon axial loading at low temperature. Pseudo-elasticity appears as load induced austenite-martensite transitions at high temperature. The shape memory effect is represented by temperature induced martensite-austenite transitions of the de-twinned, martensitic chain.

Our chain-model is motivated by works on elasto-plasticity that make use of snap springs for modeling the load/strain behavior of one lattice element [3, 4]. While snap springs are bi-stable and cold elements, the crystals in our MD model are tri-stable and thermalized. Thus the MD simulations with the chain qualitatively represent a thermo-mechanical material.

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Keywords: Atomistic simulation, phase stability in solids, phase transitions, martensitic transformation, shape memory alloys

Interaction of point defects in ferroelectrics: parameter identification and simulation. **Oliver Goy** (TU Darmstadt, Germany), Ralf Müller (TU Darmstadt, Germany), Dietmar Gross (TU Darmstadt, Germany) GA/CT3252/007

Ferroelectric materials are used in a wide field of applications and can be found in actuators, sensors and in electronic devices. During the high number of mechanical and electrical load cycles to which the material often is exposed, fatigue phenomena may occur. This involves degradation of the material and a decrease of the electromechanical coupling capability. The causes are assumed to be ionic and electronic charge carriers, later modelled as point defects, which interact with each other, with microstructural elements in the bulk and with interfaces. Accumulation of defects can primarily lead to degradation, or finally to mechanical damage and dissociation reactions.

In order to get a better understanding of the defect accumulation processes, a model based on material forces is used to simulate the interaction of defects in periodic and in infinite cells. Applying reasonable kinetic laws, defect migration is simulated in a deterministic way in order to obtain a general tendency of defect formations. The transversally isotropic material is modelled with linear electromechanical coupling.

The defect parameters used in the continuum model are obtained by fitting the results of molecular dynamics (MD) simulations to the continuous spatial fields. Transferring data from the atomic to the continuum level is a field of active research and no unique solution can be presented. On the atomic level, Coulomb–interaction causes a displacement field incompatible to an elastic solution. In order to solve this difficulty, the volume expansion or contraction of a volume around the defect is used to determine defect parameters.

Stability analysis of thermodynamic lubrication problems in journal-bearing devices. **José Durany** (Universidad de Vigo, Spain), Fernando Varas (Universidad de Vigo, Spain), José Pereira-Pérez (Universidad de Vigo, Spain) GA/CT2456/007

The analysis of thermal effects in hydrodynamic lubrication is very important because the technical advance requires more and more trustworthy and effective industrial devices. In this way, the coupled problem is given by the viscosity influence in the hydrodynamic equation, and the velocity field obtained from pressure gradients that it is introduced in the energy equation. Additionally, the bush and shaft thermal exchange with the external environment must be included in the model.

For the numerical solution a finite-element method (FEM) for the hydrodynamic Reynolds equation with a cavitation model of Elrod–Adams is applied (Durany–Pereira–Varas (2006_a)). Next, the energy equation in the lubricating film is solved by a cell–vertex volume method (Morton–Stynes–Süli (1997)). The advantage of this method lies in the possibility of retrieving second-order convergence. The analysis also takes into account the heat transfer by conduction within the bush and shaft. In the first case the bushing temperature distribution is computed by using a P1 collocation boundary-element method. The extension of this model to describe the evolution problem is quite straightforward (Durany–Pereira–Varas (2006_b)), incorporating a transient term in Elrod–Adams equation and in energy equations. Nevertheless, the adaption of the boundary-element scheme used for the thermal model in the bush is not so easy. A combination of boundary-element and dual-reciprocity methods (DRM) can be used to obtain time-stepping algorithms.

Additionally, a model describing the movement of the shaft must be provided. If the shaft is considered as a rigid body this model will consist of an ODE system (relating acceleration of the center of gravity and the external and pressure loads).

Our numerical experiments of mechanical stability try to clarify both the position of the neutral stability curve and the kind of instabilities by analysing the dynamical response of a journal-bearing system based on the Elrod–Adams equation (that do not impose the location of the cavitated region).

Mathematical and physical aspect of the solution of the Cauchy problem to the system of equation describing nonlocal model of propagation of heat with finite speed. **Gawinecki Jerzy Gawinecki** (Military University of Technology, Warsaw, Poland), Józef Rafa (WAT Military University of Technology, Poland), Jaroslaw Lazuka (Institute of Mathematics and Cryptology Military U, Poland) GA/CT1324/007

A new system of equations describing nonlocal model of propagation of heat with finite speed in three-dimensional space has been considered. At first, using Cagniard de Hoop's method, we constructed the fundamental solution for this system of equations. Basing on the constructed fundamental solution, we obtained the explicit formula for the solution of the Cauchy problem for this system of equation and next, applying the method of Sobolev spaces, we have got the $L^p - L^q$-time

decay estimate for the above solution of the Cauchy problem. Basing on the desired $L^p - L^q$-time decay estimate for the solution of the Cauchy problem for the linearized system of equation, we can prove the existence of the global (in time) solution to the Cauchy problem for the nonlinear system associated with linear one.

Deviation of macroscopic properties as a consequence of nano-scopic surface. **Jens Kruschwitz** (Universität Duisburg-Essen, Germany), Max Setzer (Universität Duisburg-Essen, Germany)

GA/CT3668/007

Every macroscopic model is based on properties of the microstructure of the material which can be deviated from assumptions or basic research measurements. In macroscopic physics and chemistry bulk properties are dominant. That is, these depend on mass and volume as extensive parameters. From a scale below $\approx 0.1\,\mu m$ surface physics and chemistry become all-dominant. Therefore, at least two size regions must be handled separately. We studied experimentally the surface interaction in hardened cement paste between solid gel and nanoscopic pores filled either with air or pore water. The physical interpretation shows that the interaction is so intensive that solid and water cannot be handled separately. Therefore, we characterize the system by naming it solid-liquid gel-system. The aim of this contribution is to connect these forces by a multi-scaling theory with the macroscopic phenomena like isothermal or frost shrinkage.

08, Short Communications

GA/CTS4342/08: Atomic- and dislocation-based approaches.

Organiser: Thomas Böhlke (Universität Karlsruhe, Germany)
Co-organiser: Bob Svendsen (Universität Dortmund, Germany)

A novel quasicontinuum method for the seamless transition from atomic to continuum length scales and its application to nanoindentation of single-crystalline materials. **Bernhard Eidel** (TU Darmstadt, Germany), Alexander Stukowski (TU Darmstadt, Germany) GA/CT2394/008

This contribution presents a novel multiscale approach aiming at a seamless transition from the atomic to the continuum description of crystalline solids at zero temperature, which is closely related to the quasicontinuum (QC) method.

A key criterion for the construction of a concurrent multiscale methodology is the seamless transition between different length scales. The original QC formulation[1] does not satisfy this requirement due to nonphysical ghost forces arising at the atomic/continuum interface. These are caused by a general mismatch between a local energy computation in the coarse-grained region (using the Cauchy–Born rule) and the nonlocal atomic description.

The new multiscale approach avoids such ghost forces by sticking to a single fully nonlocal description that is applied in all regions of space. Starting from a lattice statics model, dispensable atomic degrees of freedom are replaced by kinematic constraints as has been done[2]. The total potential energy is approximately computed using a sampling scheme with adaptive resolution. In contrast to[2], where approximate nodal forces are computed, this new approach retains a well defined total potential resulting in conservative forces and a symmetric stiffness matrix. Thus, the present ansatz endows the theory with a variational structure. Moreover, it allows the direct application of standard minimization methods and guarantees the existence of an equilibrium state provided that the total potential has a local minimum. The novel QC method is applied to nanoindentation into an fcc single crystal to showcase its performance.

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An atomic-interaction-based continuum model for computational multiscale contact mechanics. **Roger Sauer** (University of California, Berkeley, USA), Shaofan Li (University of California, Berkeley, USA) GA/CT2827/008

A computational multiscale contact mechanics model is proposed to describe the interaction between deformable solids based on the interaction of individual atoms or molecules. The model is formulated in the framework of large deformation continuum mechanics and is based on the homogenizing of the discrete description of a large assembly of interacting atoms. The atomic interaction is distinguished into two different cases: the interaction of atoms within a small neighborhood, and the interaction of atoms over large distances. The former furnishes a constitutive relation for the continuum, like the Cauchy-Born rule, while the latter is used to model the interaction, like contact and adhesion, between distinct bodies. The proposed multiscale contact model is formulated as a variational principle and implemented within the finite element method. Three different implementations are proposed, designed to maintain computational efficiency as the length scale increases. In this respect it is shown, that the proposed contact model can lead to a seamless transition between nanoscale contact mechanics, as modelled by molecular dynamics, and macroscale contact mechanics, as modelled by continuum mechanics.

The multiscale contact model is fully normalized in order to determine its characterizing model parameters. These are used to analyze the physical and numerical behavior of the contact model. In particular the scaling of the model is investigated and studied over a wide range of length scales and material properties. The consistency and accuracy of the three formulations is analyzed by a simple contact patch test. Several numerical examples are used to illustrate the applicability of the proposed model to micro/nano-scale contact/interaction problems. By using a second level of homogenization, it is finally shown, that the proposed model can be applied to macroscale contact problems.

Variational approach to formation of mis-oriented micro-structures in plastic deformation. **Radan Sedláček** (TU München, Germany), Jan Kratochvíl (Czech Technical University, Prague, Czech Republic), Martin Kružík (Czech Academy of Sciences, Czech Republic), Christian Krempaszky (TU München, Germany) GA/CT2152/008

The formation of misoriented dislocation cells in the course of plastic deformation is one of the most distinguished features of the deformation-induced microstructures. The cells are separated by dislocations assembled in boundaries that accommodate the resulting mismatch in lattice rotations. The formation of the misoriented cells is explained within the framework of continuum mechanics as a result of the trend to reduce the energetically costly hardening in multislip by locally decreasing the number of active slip systems by local lattice rotations. This explanation is broadly accepted and supported by Finite Element simulations of crystal plasticity where a dominant secondary hardening leads to a grain subdivision. However, an analytically tractable model of the misoriented cell formation that takes into account dislocation mechanisms responsible for the size of the cells and orientation of the boundaries is still lacking.

We present a model of an infinite crystal deformed in plane strain by symmetric double slip, where the plastic strain is carried by straight, parallel edge dislocations. The variational formulation of the incrementally-linear rigid-plastic approximation to crystal plasticity establishes a link to the mathematical theory of non-convex energy minimization. It is shown that a microstructure consisting of a superposition of two periodically arranged sets of parallel deformation bands separated by sharp dislocation boundaries tends to minimize the energy functional by developing a finer and finer microstructure [Sedláček and Kratochvíl, Z. Metallkunde 96 (2005) 602]. The proof that the deformation bands separated by sharp boundaries are energetically favourable has been furnished only recently [Kružík *et al.* in preparation]. The proof relies on the quadratic structure of the corresponding energy functional expressed in terms of the deformation gradient and on the relaxation theory of the variational calculus [Ball and James, Arch. Rat. Mech. Anal. 100 (1987) 13]. In a further development, by considering dislocation interactions, we introduce an internal length-scale into the model that leads to a finite size of the cells as well as to a specific orientation of the deformation bands [Kratochvíl *et al.*, Phys. Rev. B, submitted].

Short-range interactions in the continuum dislocation-based model of plastic deformation. **Cornelia Schwarz** (TU München, Germany), Radan Sedláček (TU München, Germany), Ewald Werner (TU München, Germany) GA/CT2182/008

We present the latest development of the continuum dislocation-based model of plastic deformation at the micrometer scale that was enhanced by considering short-range dislocation interactions.

The model describes the size-dependent behaviour of materials with microstructure (e. g. composites) or of micrometer-scaled samples (e. g. thin films). The size-dependence in the original model [Sedláček *et al.*, Phil. Mag. 83 (2003) 3735] was solely due to the non-locality related to the line tension of the curved dislocations. The line-tension represents the strongest and always present short-range dislocation interaction. To overcome the problem of averaging that appears in the continuum theory of dislocations, the concept of single-valued dislocation fields was introduced. Utilizing crystal plasticity, the description of the evolving single-valued fields of continuously distributed curved dislocations has been coupled with a small-strain continuum mechanics framework. The coupling accounts for the long-range elastic dislocation fields. The resulting system of partial differential equations is a convection-diffusion problem with dominating convection that is solved numerically by means of the so-called dislocation-Lagrangian method developed by Sedláček *et al.* [Phil. Mag. accepted]. This is a numerical technique that enables a stable solution of the considered problem by tracking individual segments of representative dislocations in time.

Recently, the model has been enhanced by considering other short-range dislocation interactions, namely, the mutual interactions between dislocations. To this end, by generalizing the result of Groma *et al.* [Acta Mater. 51 (2003) 1271], we consider gradients of dislocation density perpendicular to the local dislocation line direction. The resulting back stress modifies the size dependence of the modeled material behaviour and improves the numerical features of the resulting convection-diffusion problem.

We present results of several applications of the enhanced model which has been implemented for applications to two-dimensional plane-strain problems, where the continuum-mechanics part is solved by the Finite Element Method. Physical as well as mathematical consequences of the introduction of the back stress representing the short-range dislocation interactions in the model will be discussed.

On the relevance of discreteness in the continuum modeling of dislocation interactions. **Anish Roy** (TU Eindhoven, The Netherlands) GA/CT3194/008

In metals, plastic deformation is mainly attributed to the motion of a large number of discrete defects, namely dislocations. Continuum frameworks of dislocation based plasticity are gaining prominence in the mechanics research (Acharya and Bassani, 2000; Arsenlis et al., 2004). In a continuum setting, dislocation distributions are represented by an averaged continuous description of signed dislocation density. The long range stress interactions are taken care of in a mechanistically rigorous sense. However, the short range interactions between the individual dislocations are either neglected or modeled phenomenologically (Acharya and Roy, 2006).

Completely averaging out the short range interactions bears its ramifications in the overall response of plastic behavior in crystals, for instance in the prediction of pile-ups at grain boundaries. It is realized that these interactions play an important role in dislocation evolution and the lack of collective accounting of such interactions becomes quite significant. Groma et al., 2003 realized the importance of correct characterization of the short range interactions in a continuum setting and attempt to do so in a statistical mechanics framework.

We use a deterministic analysis of an idealized dislocation pile-up against an obstacle to study the current shortcomings in crystal plasticity frameworks. It is realized that the underlying discreteness of the dislocation pattern matters but there is a directional dependence of the discreteness. Based on these observations we attempt to develop a rigorous, physically motivated, continuum description of dislocation mechanics which accounts for both the long-range and short-range interactions accurately.

GA/CTS4403/08: Homogenisation.

Organiser: Stefan Diebels (Universität des Saarlandes, Germany)
Co-organiser: Bob Svendsen (Universität Dortmund, Germany)
Co-organiser: Thomas Böhlke (Universität Karlsruhe, Germany)

Mechanical anisotropies of textured polycrystalline metals. **Thomas Böhlke** (Universität Karlsruhe, Germany), Katja Jöchen (Universität Karlsruhe (TH), Germany) GA/CT2641/008

Polycrystalline metals are random heterogeneous media the microstructure of which can be described by n-point probability functions[3]. If these functions are translationally invariant or rotationally invariant the material is either called statistically homogeneous or statistically isotropic. Anisotropies of the macroscopic mechanical behavior are caused by statistically non-isotropic microstructures. They are of significant importance in mechanical engineering as well in materials science. In the presentation we discuss the combination of the aforementioned statistical approach with classical concepts of continuum mechanics. Special emphasis is given to bounds and estimates of effective mechanical properties based on orientational averages (see e.g.,[1,2]). Both, elastic and inelastic properties are considered.

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[3] Torquato, S; Random Heterogeneous Materials: Microstructures and Macroscopic Properties. Springer, 2002.

Micromechanical and macroscopical hardening modeling as basis for the realistic simulation of sheet forming processes with complex strain-path changes. **Vladislav Levkovitch** (Universität Dortmund, Germany), Bob Svendsen (Universität Dortmund, Germany) GA/CT3302/006

Sheet metal forming involves large strains and severe strain-path changes. Large plastic strains lead in many metals to the development of persistent dislocation structures resulting in strong flow anisotropy. This induced anisotropic behavior manifests itself in the case of a strain path change by very different stress-strain responses depending on the type of the strain-path change. While many metals exhibit a drop of the yield stress after a load reversal, some metals show an increase of the yield stress after an orthogonal strain-path change (so-called cross hardening). To model the Bauschinger effect, kinematic hardening has been successfully used for years. However, the usage of the kinematic hardening leads automatically to a drop of the yield stress after an orthogonal strain-path change contradicting tests exhibiting the cross hardening effect. Another effect, not accounted for in the classical elasto-plasticity, is the difference between the tensile and compressive strength (SD effect), exhibited e.g. by some steel materials. In this work we first present a micromechanical model

that takes into account the evolution of polarized dislocation structures on the grain level, the non-Schmidt effect for the dislocation slip resistance and texture evolution. The micro-macro transition is performed via the Taylor hypothesis. The model is used to investigate the evolution of the yield surface. From these investigations we derive a macroscopic model that considers besides the movement of the yield surface and its proportional expansion, as it is the case in conventional plasticity, also the changes of the yield surface shape (distortional hardening) and accounts for the pressure dependence of the flow stress. All these additional attributes turn out to be essential to model the stress-strain response of high-strength steels subjected to non-proportional loading. The model is applied to predict the spring-back in processes with complex strain-path changes.

Non-local numerical homogenization scheme. **Ralf Jaenicke** (Universität des Saarlandes, Germany), Holger Steeb (Universität des Saarlandes, Germany), Stefan Diebels (Universität des Saarlandes, Germany) GA/CT2158/008

The numerical treatment of multiscale models is of built on the so-called FE^2 concept; i.e., a testing volume consisting of a certain microstructural elements is attached to the integration point of a macroscopic finite element model. The local strain at the integation point is mapped onto the boundary of the testing volume, and, after solving the local boundary value problem, the macroscopic stresses are computed by a homogenization procedure applied to the local problem. In the present contribution the testing volume is assumed to be of small but finite size and, therefore, the local boundary value problem is directly derived from the displacement solution within the finite element. The stresses are computed by an appropriate homogenization scheme and extrapolated to the macroscopic integraton points. In the limit, if the testing volume reaches the size of the finite element, the proposed method becomes similar to domain decomposition methods and the local structure is resolved explicitly.

Towards the computational homogenization of discrete microstructures. **Sarah Ricker** (TU Kaiserslautern, Germany), Andreas Menzel (Universität Siegen, Germany), Paul Steinmann (TU Kaiserslautern, Germany) GA/CT2270/008

The past years have been marked by a growing significance in multi-scale mechanics. This interest is founded on the fact that the concept of pre-assumed (overall) material parameters, or rather constitutive relations, cannot reflect all features of a material with underlying (heterogeneous) continuous or discrete microstructure.

The computational homogenization scheme provides an effective tool to bridge different length scales between the micro- and the macro-level for both continuous and discrete microstructures.

The considered macroscopic specimen is studied by means of finite-element methods, while the associated underlying microscopic setting in each Gauss point is – in the discrete case at hand – identified with so-called mass-spring networks. Furthermore, the influence of different boundary conditions on the micro-level, e.g. linear displacements, periodic displacements and antiperiodic tractions, or constant tractions, on the behavior of the macroscopic specimen is investigated.

Computational micro–macro transitions at large strains for curvilinear physical directions. **Rafael Grytz** (Ruhr-Universität Bochum, Germany), Guenther Meschke (Ruhr-Universität Bochum, Germany) GA/CT2360/008

Biological tissues such as those involved in the eye, heart, veins or arteries are heterogeneous on one or another spatial scale and can undergo very large elastic strains. Frequently, these tissues are characterized by shell-like structures at the macroscopic scale and the physical material directions follow curvilinear paths. We consider a homogenized macro-continuum formulated in curvilinear convective coordinates with locally attached representative micro-structures. Micro-structures attached to different macroscopic points are assumed to be rotated counterparts according to the curvilinear path of the physical material directions at the macro-scale. The solution of such multi-scale problems according to the computational homogenization scheme[1,2,3] would need a different RVE at each macroscopic point.

The goal of this paper is to use the same initial RVE at each macroscopic point by generalizing the computational homogenization scheme to a formulation considering different physical spaces at the micro- and macro-scale. The deformation and the reference frame of the micro-structure are assumed to be coupled with the local deformation and the local reference frame at the corresponding point of the macro-continuum. For a consistent formulation of micro-macro transitions *physical reference directions* are defined on both scales, where the macroscopic one follows a curvilinear path. To formulate the generalized micro-macro transitions in absolute tensor notation the operations *scale-up* and *scale-down* are introduced.

The proposed formulation considering curvilinear physical directions at the macro-scale as well as geometrical and material nonlinearities is demonstrated by means of a multi-scale analysis of a spherical shell structure. This example is characterized by a finite-element discretization of the macro-continuum by means of a bilinear finite shell element with a quadratic kinematic assumption in thickness direction[4], where the integration through the thickness is carried out numerically. A finite element discretization of the same initial micro-structure is attached to each integration point of these macro-elements. The micro-structure is modeled by means of trilinear brick elements.

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On the simulation of textile-reinforced concrete using a multi-scale approach. **Ingolf Lepenies** (TU Dresden, Germany), Mike Richter (TU Dresden, Germany), Bernd Zastrau (TU Dresden, Germany) GA/CT3351/008

Textile reinforced concrete (TRC) is a composite of rovings (bundles of endless fibers) and fine grained concrete which is used in the field of civil engineering for the fabrication of new structural elements and the strengthening of existing constructions.

Experimental investigations on textile reinforced concrete samples show very complex failure mechanisms on different length scales. Therefore descriptions on the micro, meso and macro scale are introduced. The presentation shows a hierarchical material model of textile reinforced concrete.

Due to the small dimensions of the filaments and the partial impregnation of the roving within the cementitious matrix a detailed study of the load transfer mechanism on a micro scale under consideration of individual filaments and adhesive cross linkages has been investigated.

To simulate the material behavior of textile reinforced concrete on a larger scale a homogenization is required to reduce the numerical costs. Therefore idealized roving models are developed. The aim of the micro/meso homogenization is an effective roving model to simulate the relevant load transfer mechanisms.

On the so called meso scale a multi-axial textile structure made rovings is modeled. This allows the evaluation of effective material parameters of the analyzed domain in three dimensions by means of numerical and analytical homogenization techniques. One benefit of the used model is the determination of the initial and induced type of material symmetry.

Based on this hierarchical material description and the scale bridging between the different scales a multi-scale Finite-Element-Methods (MS-FEM) of a sequential and integrated type are used.

GA/CTS4405/08: Foams and composites.

Organiser: Tom-Alexander Langhoff (Universität Karlsruhe (TH), Germany)
Co-organiser: Bob Svendsen (Universität Dortmund, Germany)
Co-organiser: Thomas Böhlke (Universität Karlsruhe, Germany)

Numerical analysis of uncertainties in the effective material behaviour of disordered structural foams. **Jörg Hohe** (Fraunhofer IWM Freiburg, Germany), Volker Hardenacke (Fraunhofer IWM Freiburg, Germany) GA/CT1844/008

Solid foams are important materials in many fields of modern lightweight construction. The main advantages of this class of materials is their low specific weight in conjunction with their ability to perform additional, non-mechanical functions such as e.g. heat insulation. Disadvantage is the disordered random microstructure leading in many cases to a distinct variability in the macroscopic material parameters.

The present contribution is concerned with a numerical analysis of the uncertainties in the structural response of three-dimensional structural foams with partially open cells. The effective thermo mechanical material response is determined by means of an energy based homogenization procedure using the finite element method for the microstructural analysis. Stochastic effects in the geometry and topology of the microstructure are treated by means of a Monte-Carlo approach in conjunction with a repeated analysis of small-scale representative volume elements with prescribed relative density and prescribed cell size distribution. The results are evaluated by stochastic methods in order to determine the probability distribution of the effective material parameters. Meso scale variations in the relative density and the cell size distribution are included by a direct stochastic approach.

The approach is applied to the effective elastic, plastic and thermal material parameters of aluminum foams with different nominal relative densities. Strong effects of the microstructural disorder are observed especially with respect to the mechanical strength of the material on the macroscopic level, where both, the expectation and the variance of the material properties are strongly affected by the microstructural disorder. The numerical results are found in good agreement with experimental data from the literature.

Local stochastic analysis of the effective material response of disordered two-dimensional model foams. **Volker Hardenacke** (Fraunhofer IWM Freiburg, Germany), Jörg Hohe (Fraunhofer IWM Freiburg, Germany) GA/CT1932/008

Solid foams are important materials in many fields of modern lightweight construction. The main advantages of this class of materials is their low specific weight in conjunction with their ability to perform additional, non-mechanical functions such as e.g. heat insulation. Disadvantage is the disordered random microstructure leading in many cases to a distinct variability in the macroscopic material parameters.

In order to comply with this problem, a stochastic homogenization procedure is proposed. The procedure is based on the multiple analysis of a medium scale representative volume element consisting of a relatively low number of cells. The representative volume element is subdivided into a number of (non representative) subcells, each consisting of a single cell wall intersection and the corresponding cell walls. For each of the subcells, the average stress and strain states are determined using a strain energy based homogenization procedure. For comparison, an analysis based on the randomization of a regular periodic microstructure is performed.

The disordered microstructure for the representative volume element are determined automatically based on a Voronoi tessalation of the area of the RVE. Different approaches are used, including Γ- and δ-Voronoi techniques, closed-packing-of-spheres models in conjunction with a Laguerre-Voronoi approach, foam evolution models and optimization strategies in order to obtain realistic computational models.

The results of the homogenization analysis are evaluated by means of stochastic methods. Distinct effects of the microstructural disorder are observed. Compared to an idealized regular periodic foam model, the microstructures in general become weaker, if the microstructural disorder is taken into account.

Constitutive modelling of interpenetrated metal ceramic composites with evolving anisotropy. **Felix Fritzen** (Universität Karlsruhe (TH), Germany), Eckart Schnack (Universität Karlsruhe (TH), Germany) GA/CT2141/008

Several phenomenological aspects concerning the constitutive modelling of class interpenetrated $Al - Al_2O_3$ metal-ceramic composites undergoing quasistatic thermo-mechanical loading are presented. The heterogeneous a-periodic microstructure of the material motivates a two-scale incremental treatment of its deformation behaviour. The initial phase of constitutive modelling is devoted to phase-specific formulation of the constitutive response on micro scale in terms of incremental quasihyperelastic potentials [1]. In this context, the inelastic behaviour of the metal phase is described by a J_2-flow rule with isotropic exponential hardening and a multiplicative thermal softening function. Latter accounts for the thermal softening of Aluminium at high temperatures. A smeared crack model is used to depict the quasi brittle damage behavior of the Al_2O_3 ceramic constituent following the conceptual line pointed out in [2]. This model allows for a developping anisotropy of the mechanical properties of the ceramic constituent due to a degradation of the material stiffness tensor by the onset of inelasticity. Thermodynamical consistency is granted for both models. Unilateral effects are also considered in the constitutive model. At this stage both models are limited to rate-independent deformation processes.

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Zweiskalensimulation von Schädigungsprozessen in unidirektional faserverstärkten Verbundwerkstoffen. **Benjamin Köster** (Universität Kassel, Germany) GA/CT2227/008

Bei der Beanspruchung von Verbundbauteilen bis in den Bereich der Werkstoffschädigung handelt es sich um komplexe, gekoppelte Vorgänge auf unterschiedlichen Längenskalen. Die mittlerweile verfügbare Rechnerkapazität ermöglicht die gleichzeitige Mehrskalensimulation derartiger Prozesse. Bei der hier unternommenen Zweiskalensimulation von Faserverbundstrukturen wird die Makroskala durch die Ebene der strukturmechanischen Bauteile oder Bauteilkomponenten definiert. Die Mikroskala ist durch die typischen Abmessungen der Heterogenitäten des Verbundwerkstoffe bestimmt. Das Ziel der gekoppelten Mikro-Makro-Analyse ist die realitätsnähere strukturmechanische Simulation auf Basis einer detaillierteren Betrachtung der Vorgänge auf der Mikroebene des Werkstoffs. Die Makroskala wird durch übliche Ansätze der FE-Methode modelliert. Zur Beschreibung der Mikroskala wir eine repräsentatives Volumenelement (RVE) des inhomogenen Gefüges betrachtet. Die Mikrofelder der Spannungen und Verzerrungen im RVE sind die Lösung einer Randwertaufgabe, die für das Volumenelement formuliert wird. Die verallgemeinerte Methode der Zellen (engl. Generalized Method of Cells, kurz: GMC) liefert eine Näherungslösung für das diskretisierte Verformungsfeld im RVE. Als geometrische Randbedingungen dienen die Verzerrungen der Makroskala. Unter Einbringung geeigneter Konstitutivmodelle in das Zellenmodel für die Phasen und deren Verbund können dann die zu den Makrodehnungsprozessen gehörigen Mikrofelder der Verzerrungen und Spannungen berechnet werden. Das makroskopische Werkstoffverhalten wird durch einen prozessabhängigen Konstitutivtensor beschrieben, der die Abbildung zwischen den volumengemittelten Mikrofeldern der Spannungen und Verzerrungen im repräsentativen Volumenelement leistet. Das mikromechanische Modell liefert als Ergebnis sowohl den konsistent linearisierten, konstitutiven Tensor als auch die makroskopische Spannungsantwort in jedem numerischen Integrationspunkt des Makrostrukturmodells. Der Homogenisierungsalgorithmus der Zellenmethode läuft simultan zur FE-Analyse ab.

Study of wave dispersion in periodic composites by higher-order asymptotic homogenization method. **Vladyslav Danishevskyy** (Prydniprovska State Academy, Ukraine), Igor Andrianov (RWTH Aachen, Germany), Vladimir Bolshakov (Prydniprovska State Academy, Ukraine), Dieter Weichert (RWTH Aachen, Germany) GA/CT2871/008

In the present work an application of the higher-order asymptotic homogenization method (AHM) to the study of wave dispersion in periodic composite structures is considered. It should be noted that the most significant and practically important phenomena caused by the heterogeneity of the composite media arise in dynamic problems. When the wavelength of a travelling signal becomes comparable to the size of heterogeneities, successive reflections and refractions of the waves at the componentsŠ interfaces lead to the formation of a complicated sequence of so called pass and stop frequency bands. In this case the composite plays a role of a discrete frequency filter.

As illustrative examples we study propagation of harmonic elastic waves in a layered composite (one-dimensional problem allowing the exact analytical solution) and in a fibre-reinforced composite with the square array of cylindrical inclusions (two-dimensional problem). The asymptotic homogenization schemes are developed and the higher-order macroscopic wave equations are derived. Analysis of the obtained solutions shows that the AHM provides a long-wave approach valid in the low frequency range. Solutions for the high frequencies are obtained on the basis of the Floquet-Bloch theorem by expanding spatially varying material properties in Fourier series and representing unknown displacement fields by infinite plane-wave (PW) expansions. However, this approach may run into convergence problems with the increase in contrast between the components properties. Eventually, we can conclude that the higher-order AHM and the PW expansions method can be treated as complementary to each other. The dispersion curves relating the wave numbers and frequencies are obtained; the pass and stop frequency bands are identified; the attenuation factors within the stop bands are evaluated.

GA/CTS4406/08: Mathematical and numerical aspects.

Organiser: Vladislav Levkovitch (Universität Dortmund, Germany)
Co-organiser: Bob Svendsen (Universität Dortmund, Germany)
Co-organiser: Thomas Böhlke (Universität Karlsruhe, Germany)

Well-posedness of infinitesimal gradient-plasticity. **Patrizio Neff** (TU Darmstadt, Germany) GA/CT2494/008

I derive a model of infinitesimal isotropic gradient plasticity. The second law of thermodynamics is modified to include an extra entropy flux. Boundary conditions for the plastic variable are nonstandard.The higher plastic gradient consists only of the dislocation density tensor. Kinematical hardening is included.The flow law turns into a second order parabolic evolution equation. Assuming monotonicity of the flow function it is possible to show well-posedness of the model in a novel Hilbert-space setting which incorporates the Dislocation density

Phase-field simulations on the interaction of ferroelectric domain structures with point defects. **Bai-Xiang Xu** (TU Darmstadt, Germany), David Schrade (TU Darmstadt, Germany), Ralf Müller (TU Darmstadt, Germany), Dietmar Gross (TU Darmstadt, Germany) GA/CT1441/008

It is suspected that point defects and their agglomerates lead to the electric fatigue in ferroelectric materials. In this work, the interaction of ferroelectric domains with point defects and their agglomerates is simulated, using a continuum phase-field model. Expanding the energy of the system by a phase separation and a domain wall contribution and regarding the polarization as an order parameter, the model has successfully revealed typical behavior of ferroelectrics. This includes the formation of domain structures, the migration of domain walls, the dielectric and butterfly hysteresis loops and the ferroelastic switching. To model point defects, such as foreign atoms and vacancies, an inelastic eigenstrain and a localized volume charge are introduced.
Calculations show the hindering effect of defects on the domain wall movement. A delay by defects in the microstructure evolution is also observed. Finally, the influence of point defects on the ferroelectric hysteresis loops is studied. It is demonstrated that the presence of defects apparently hinders the polarization switching and changes hysteresis in a characteristic manner. Results of the simulations show good agreement with experimental phenomena reported in the literature.

Homogenization of special GFRP truss-type elements. **Janko Kreikemeier** (Universität Magdeburg, Germany) GA/CT4026/008

The paper deals with the numerical homogenization of the effective material properties of special glass fibre reinforced truss type elements called Polystal Profiles. The commercial available profiles are made from longitudinal aligned glass fibres embedded in an epoxy resin. The diameters of the cross sections ranges from 1 mm to 16 mm. Originally designed for the strain release of submerged lying optical cables we see other fields of application like the reinforcement of hollow section profiles to exploit the material properties and to improve the loading behaviour. For this purpose we used the method of representative volume element (RVE) to estimate the effective material properties by applying periodic boundary conditions (PBC). To create the RVE a FORTRAN program was developed to get a RVE with a randomly fibre arrangement above the cross section. Furthermore an ANSYS script was created for the meshing and the application of the PBC on the RVE automatically. The obtained results are discussed with respect to experimental values of the longitudinal Youngs-Modulus estimated in earlier works.

Lower-semicontinuity result for the two-scale convergence. **Mahdi Boukrouche** (Université Saint-Etienne, France) GA/CT2533/008

The aim of this talk is to prove the following result, using some results on subdifferential and regularization of convex functions: Let $\Omega \subset \mathbb{R}^m$ an open bounded domain, $Y = [0,1]^m$, and $\varphi : \Omega \times \mathbb{R}^m \times \mathbb{R}^n \to \mathbb{R}$ such that the following hypotheses hold:
(H1) $\varphi(x, \cdot, \cdot)$ is continuous a.e. for $x \in \Omega$,
(H2) $\varphi(\cdot, y, z)$ is measurable for all $(y, z) \in \mathbb{R}^m \times \mathbb{R}^n$,
(H3) $\varphi(x, \cdot, z)$ is 1-periodic in y,
(H4) $\varphi(x, y, \cdot)$ is convex in z,
(H5) $\exists C_1 > 0$ and $\exists C_2 \in L^2(\Omega)$ such that
$|\varphi(x, y, z)| \le C_1 \|z\|^2 + C_2(x) \quad a.e. \quad x \in \Omega \quad \forall (y, z) \in \mathbb{R}^m \times \mathbb{R}^n$

Let u^ε in $(L^2(\Omega))^n$ which two-scale converges to some u in $(L^2(\Omega \times Y))^n$, and φ such that (H1)–(H5) hold. Then we have

$$\liminf_{\varepsilon \to 0} \int_\Omega \varphi(x, \frac{x}{\varepsilon}, u^\varepsilon(x)) dx \ge \int_\Omega \int_Y \varphi((x, y, u(x, y)) dy dx .$$

Joint Work with Ionel Ciuperca, Institut Camille Jordan Université Lyon1, UMR 5208. (Email: ciuperca@math.univ-lyon1.fr)

On dispersive stability of Hamiltonian systems on lattices. **Carsten Patz** (Weierstraß-Institut Berlin, Germany) GA/CT2890/008

We study the long-time dynamics of *oscillations in lattices of infinitely-many particles* interacting via certain nonlinear potentials. In particular we consider the Klein-Gordon system on the infinite chain and the two dimensional lattice. The aim is to proof *dispersive stability* of such Hamiltonian systems analogously to results known for PDEs.

To do so we first recapitulate the dynamics of linear Hamiltonian systems on an infinite chain and give optimal decay rates based on the dispersion relation. We will also discuss the two dimensional lattice with nearest-neighbour interaction where more complicated singularities occur.

Based on this we proof that if the nonlinearity is weak enough, the Klein-Gordan system shows a similar behaviour like its linearisation.

Up-scaling in nonlinear thermal-diffusion problems. **Claudia Timofte** (University of Bucharest, Romania) GA/CT4184/008

The general question which will make the object of this paper is the homogenization of some nonlinear problems arising in the modelling of thermal diffusion in a two-component composite. We consider, at the microscale, a periodic structure formed by two materials with different thermal properties. We shall consider two situations: in the first one, we assume that we have some nonlinear sources acting in both components and that at the interface between our two materials the temperature and the flux are continuous, while in the second problem we shall address here, we assume that the flux is still continuous, but depends in a nonlinear way on the jump of the temperature field. In both cases, since the characteristic sizes of these two components are small compared with the macroscopic length-scale of the flow domain, we can apply an homogenization procedure.

Using the so-called energy method introduced by L. Tartar, in the first case we can prove that the limit problem will be a new nonlinear elliptic boundary-value problem with extra zero-order terms capturing the effect of the nonlinear sources acting in our two parts of the domain. The asymptotic behavior of the solution of the second problem will be governed by a new nonlinear system, similar to the famous Barenblatt's model, with extra zero-order terms capturing the effect of the interfacial barrier and of the nonlinear sources.

GA/CTS4404/08: Phenomenological and field approaches.

Organiser: Patrizio Neff (TU Darmstadt, Germany)
Co-organiser: Bob Svendsen (Universität Dortmund, Germany)
Co-organiser: Thomas Böhlke (Universität Karlsruhe, Germany)

Comparison of phenomenological theories with physically-based theories of plasticity. **Vladimir Shneider** (Dnipropetrovs'k National University, Ukraine), Yuriy Chernyakov (Dnipropetrovs'k National University, Ukraine) GA/CT619/008

The theory of plasticity, including micro strains [1,2], considers heterogeneity of representative macro volume of polycrystalline material by introduction of micro particles with various yield stresses and various directions of micro plastic deformation. These micro particles can interact and affect macroscopic stress-strain state. In theory the generalization of physical approaches to the description of plastic deformation (Schmid law) realized and invariant approach displaying transition to higher scale level (from a level of dislocation sliding up to a level of micro plastic deformation of grain) is applied. It was shown [2], that the theory of micro strains is reduced to many known *physical* theories of plasticity in special cases. In this paper comparison of the theory of micro strains with the theories based on physically reasonable slip mechanisms of plastic deformation is carried out. Benefits and shortcomings of the offered invariant approach are analyzed.

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Energy functionals for microstructured multi-phase materials. **Tom-Alexander Langhoff** (Universität Karlsruhe (TH), Germany), Thomas Böhlke (Universität Karlsruhe, Germany), Eckart Schnack (Universität Karlsruhe (TH), Germany) GA/CT2197/008

Many state-of-the art materials (e.g., carbon fibre reinforced carbon, CFC) show a multi-phase and a multi-scale character. For describing the material response, energetic models have been developed for a wide range of problems in many of which the energy functionals are no longer convex [1]. Restrictions on the energy functionals arise in order to obtain existence results for rate-independent systems [2]. In this contribution, we propose an energetic model for describing the thermomechanical response of CFC based on the influence of the microstructure on different length scales [3]. The different phases are given by different textures of the deposited pyrolytic carbon [4]. Based on experimental observations using transmission electron microscopy [5] showing sharp interfaces between the different phases, an interfacial part relaxing the total free energy is included in the energy functional. Further restrictions to the energy functional result from homogenisation to macroscale and phase transformations that possibly occur especially due to thermal loading.

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[3] T.-A. Langhoff, E. Schnack; Energetic modelling for carbon fibre reinforced carbon, *Proceedings of Applied Mathematics and Mechanics*, submitted.

[4] V. De Pauw, B. Reznik, S. Kalhöfer, D. Gerthsen, Z.J. Hu, K.J. Hüttinger; Texture and nanostructure of pyrocarbon layers deposited on planar substrates in a hot-wall reactor, *Carbon* **41**, 71–77, 2003.

[5] B. Reznik, D. Gerthsen; Microscopic study of failure mechanisms in infiltrated carbon fiber felts *Carbon* **41**, 57–69, 2003.

A variational formulation of non-local materials with microstructure based on dual macro- and micro-balances. **Fabian Welschinger** (Universität Stuttgart, Germany), Dominik Zimmermann (Universität Stuttgart, Germany), Christian Miehe (Universität Stuttgart, Germany) GA/CT4006/008

We investigate a variational setting of nonlocal materials with microstructure and outline aspects of its numerical implementation. Thereby, the current state of the evolving microstructure is described by a set of order parameters. These order parameters represent independent global degrees in addition to the macroscopic displacement field. Fokussing on so-called standard-dissipative materials, the constitutive response is governed by two fundamental functions for the energy storage and the dissipation. Based on these functions, a global dissipation postulate is introduced. Its exploitation in the sense of a Coleman method constitutes a global variation formulation of nonlocal materials, which can be related to a minimization principle. Following this methodology, we end up with coupled macro- and microscopic field equations and corresponding boundary conditions. Thereby, we observe a strict duality between a macro-balance in terms of the displacment field and a micro-balance in terms of the order parameter field. On the numerical side, we consider the weak counterpart of these coupled field equations and obtain after linearization a fully coupled system for increments of the displacement and the order parameters. Due to the underlying variational structure, this system of equations is symmetric. In order to show the capability of the proposed setting, we specify the above outlined scenario to a model problem of isotropic damage mechanics and a class of single slip crystal plasticity. The performance of the symmetric coupled formulation is demonstrated by means of a set of representative numerical examples.

Micro-roughness effects in (elasto)hydrodynamic lubrication including a mass-flow preserving cavitation model. **Sébastien Martin** (Université Paris-Sud, France), Carlos Vázquez Cendón (Universidade da Coruña, Spain), Guy Bayada (INSA Lyon, France) GA/CT3491/008

An average Reynolds equation is proposed for predicting the effects of deterministic periodic roughness of the surfaces, taking JFO mass flow preserving cavitation model and elastohydrodynamic effects into account. Thus, the influence of the roughness effects over thin films flows is studied when taking into accound several nonlinearities : cavitation phenomena, piezoviscosity of the fluid, elastic deformation of the surfaces (Hertz model) due to high peak pressures.

For this, the asymptotic model is based upon a double scale analysis approach (multiscale homogenization and periodic unfolding methods) in order to describe the micro-macro effects and derive in a rigorous way the asymptotic equations. The average Reynolds equation can be used both for the description of cavitation on a macroscopic scale in widening gap regions as well as for cavitation on the microscopic interasperity scale.

Results of numerical simulations based on the model are presented for the case of a hydrodynamically lubricated journal bearings and an elasto-hydrodynamically lubricated point contact.

Improved constitutional relations by and for multiscale models. **Heike Emmerich** (RWTH Aachen, Germany) IC/CT3306/008

Constitutional relations are of great impact in materials modeling. Their accuracy determines to a large extend the accuracy at which the the macroscopic behaviour of a material can be described in a respective continuum model approach. Since these constitutional relations themselves are usually determined at the micro- or even nanoscale, they can be understood as a *natural* link between the different scales relevant in materials modelling. In spite of this undeniable impact today's theoretical materials scientists encounter quite often the situation, that *classical* constitutive relations do longer match our precise understanding of a materials microstructure dynamics, since the latter has increased dramatically due to increased experimental accessibility over the last decade. This contribution reviews this situation in terms of mathematical approaches for several phase transition problems in complex materials. Moreover we demonstrate, how homogenization techniques can be employed to derived improved constitutional relations and use them in turn for improved macroscopic continuum model approaches.

Micromechanical interpretation of the quadratic yield function by v. Mises and Hill. **Gerrit Risy** (Universität Magdeburg, Germany), Thomas Böhlke (Universität Karlsruhe, Germany), Albrecht Bertram (Universität Magdeburg, Germany) GA/CT2334/008

Both v. Mises (1928) and Hill (1948) suggested an anisotropic quadratic yield function for a phenomenological description of the plastic behavior of anisotropic solids. Such an elementary approach to the description of mechanical anisotropy has inherent shortcomings. For example, specific experimentally observed distributions of the yield stress and the Lankford coefficient in sheet metals cannot be reproduced by the quadratic yield function.

Nevertheless, the v. Mises-Hill model is currently one of the standard anisotropic plasticity models in the context of a phenomenological setting. Here an overview concerning the properties of the v. Mises-Hill model is given. Furthermore, an interpretation of the fourth-order structure tensor is given in terms of the crystallite orientation distribution function (Böh-

lke, 2005, 2006). Based on this approach the structure tensor can be completely identified by a measurement of the crystallographic texture and of two macroscopic yield stresses.

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09, Short Communications

GA/CTS4448/09: **Flow and mixing.**

Organiser: Stefan Heinz (University of Wyoming, USA)
Co-organiser: Thomas Sattelmayer (TU München, Germany)
Co-organiser: Patrick Jenny (ETH Zürich, Switzerland)

Mixing modeling for stochastic simulations of turbulent pre-mixed flames. **Michael Stoellinger** (University of Wyoming, USA), Stefan Heinz (University of Wyoming, USA) GA/CT3149/009

Due to the exact treatment of chemical reactions, stochastic methods for turbulent reacting flow simulations have significant advantages compared to deterministic methods. The performance of stochastic methods depends essentially on the modeling of the dynamics of scalar fluctuations (the scalar mixing model). Such models involve two ingredients: changes of scalar values and the characteristic scalar time scale have to be explained. Recent developments did hardly address the latter problem: the scalar time scale is usually assumed to be controlled by the time scale of large-scale turbulent motions (which neglects the influence of chemical reactions on turbulent scalar mixing). This assumption is not justified if the characteristic length scale of scalar fields (reaction zone) is smaller than the Kolmogorov microscale of turbulence. The fact that many turbulent premixed flames of technical interest operate under such conditions leads to the need to develop more general scalar time scale models. A way to overcome this problem by adopting Direct Numerical Simulation (DNS) results will be presented in this talk. The suitability and relevance of this scalar time scale model will be shown in two ways: model predictions will be compared with DNS results and model applications to simulations of several turbulent premixed flames (Aachen flames F1-F3) will be demonstrated.

Statistical modeling of compressible turbulent channel flow. **Stefan Heinz** (University of Wyoming, USA) GA/CT2986/009

Most of the simulations of turbulent reacting flows are performed on the basis of statistical methods because of their relative simplicity. However, the latter fact is the reason for some significant problems, which limit the accuracy of these methods. A first problem is given by the fact that there are good concepts available to model the evolution of velocity and scalar fields, but to close such equations one has to provide the time scale of turbulent motions. Unfortunately, the basis for constructing such a scale-determining equation is weak because the most important term (the source rate) is unknown. A second problem is related to the modeling of wall-bounded flows, which has to be considered in most of the applications. The inclusion of the damping effect of walls is a requirement to perform accurate simulations of such flows. Unfortunately, currently applied concepts for handling this question are either not supported by direct numerical simulation (DNS), or they are not invariant under the Galilean transformation. A third problem concerns the development of solutions for the two problems described above for variable-density flows, which is relevant to turbulent combustion calculations. The relevance and modeling of compressibility effects in wall-bounded flows still represents an open question. Recently obtained DNS results of turbulent supersonic channel flow are analyzed in order to address the three problems pointed out above: the turbulence frequency production mechanism, wall damping effects on turbulence model parameters, and the relevance of compressibility effects. Limited support is found for usually applied models for the turbulence frequency production and wall damping effects. In contrast to that it is shown that turbulence frequency production mechanisms and wall damping effects may be explained very well on the basis of a frequency scaling that characterizes mean flow changes. The influence of compressibility is found to be relevant.

Turbulent boundary layer on a plate with transpiration: dynamical and thermal problems. **Igor Vigdorovich** (Moscow State University, Russian Federation) GA/CT559/009

Closure conditions are derived for turbulent boundary layer flow over a flat plate with transpiration (injection and suction) in the form of universal dependence of turbulent shear stress and heat flux on mean velocity and temperature gradients. The relations can be determined by using but two empirical functions: the velocity and temperature profiles in the turbulent boundary layer flow over an impermeable plate.

As a result, the distributions of velocity, temperature, shear stress, and transverse heat flux in an entire range of parameters and the skin friction and wall heat transfer for the case of arbitrary suction are computed by solving averaged equations under very general physical assumptions without invoking any special closure hypotheses.

Similarity laws for main dynamical and thermal quantities are established as a result of asymptotic analysis of Reynolds-averaged Navier–Stokes and heat transfer equations.

In the case of injection, velocity and temperature everywhere outside the viscous sublayer have universal distributions. For suction, the profiles of these quantities in terms of scaling variables depend on one parameter. The Reynolds tensor components, turbulent heat flux, and rms temperature fluctuation also obey one-parameter scaling laws.

Skin-friction and heat-transfer laws are established such that skin-friction and heat-flux distributions at the wall can be described by universal functions of one variable. The laws are applicable in an entire range of parameters from suction velocities corresponding to an asymptotic suction boundary layer flow to injection velocities giving rise boundary layer blow-off.

Theoretical results are in good agreement with experimental data available.

Dynamic-lift measurements of airfoils. **Gerrit Wolken-Möhlmann** (Carl von Ossietzky Universität Oldenburg, Germany), Joachim Peinke (Carl von Ossietzky Universität Oldenburg, Germany), Stephan Barth (Carl von Ossietzky Universität Oldenburg, Germany) GA/CT4028/009

We present wind tunnel measurements to investigate the dynamic stall effect like it is caused by fluctuations of the wind direction and speed. The lift is determined by the integral of pressure distribution at the wind tunnel walls while rotating the airfoil with defined angular velocity. There is an increase of lift before flow separation on the suction side occurs. The results are discussed on the background of extreme mechanical loads for blades of wind turbines.

A mixing model providing statistics of the conditional scalar dissipation rate. **Daniel Meyer** (ETH Zürich, Switzerland), Patrick Jenny (ETH Zürich, Switzerland) GA/CT1743/009

In the Reynolds-averaged scalar transport equations, the highly non-linear chemical source term can be calculated based on a transport equation for the scalar joint probability density function (PDF). Here, turbulent transport is modeled [R. O. Fox, Computational Models for Turbulent Reacting Flows, 2003]. In velocity-scalar joint PDF methods, turbulent convection is closed. In both approaches, however, molecular mixing needs to be closed by a mixing model. Even though the earliest models were already introduced in the nineteen seventies [P. A. Libby and F. A. Williams, Turbulent Reacting Flows, 1994], mixing models are still an active research area. Here, the challenge is to fulfill the different requirements deduced from the nature of molecular scalar diffusion. We recently introduced a new mixing model [D. W. Meyer and P. Jenny, Physics of Fluids, 18, 2006], which is based on parameterized scalar profiles (PSP). To every particle in the PDF simulation a one-dimensional scalar profile, represented by profile parameters, is attributed. This makes it possible to obtain statistics of spatial scalar derivatives conditioned on the scalar. When treating reacting flows, such data is of great value if laminar flamelets are used [N. Peters, Turbulent Combustion, 2000]. Here, the scalar source term depends on the conditional scalar dissipation rate. In this work, the potential of the PSP mixing model for such turbulent reactive flow computations is investigated.

Turbulent shear-layer scaling in the limit of infinite Reynolds number derived from the unsteady equations of motion. **Bernhard Scheichl** (TU Wien, Austria), Alfred Kluwick (TU Wien, Austria) GA/CT1857/009

By considering the time-mean motion, an asymptotic description of turbulent shear flows in the limit of high Reynolds numbers, conveniently carried out by adopting the method of matched asymptotic expansions, is inherently based on (a few) assumptions regarding the essential physical properties of the flow in the respective tier considered. Although this approach has substantiated some classical results as, for instance, the logarithmic law of the wall, it is, nevertheless, not completely satisfactory from a rational point of view: to this end, we first demonstrate that a rigorous application of the matching principle alone is *not* capable of deducing the aforementioned wall law in the case of boundary layer flows by taking into account the widely accepted presumption of the so-called "inviscid" nature of the fully turbulent main portion of the shear layer. Therefore, to some extent, the usual approaches turn out to be incomplete, for (i) the motivation for the assumptions commonly employed seems not stringent and, unfortunately, (ii) are, stricly speaking, insufficient for developing an asymptotic theory. To be more precise, assumptions which are usually expressed by dimensional considerations can not adequately enter the matching conditions derived from the non-dimensional form of the governing equations, which, however, is required for an asymptotic analysis. Consequently, and as is elucidated, the time-mean scaling of the asymptotic splitting of the flow has to result from an asymptotic analysis of the Navier–Stokes equations by, as the only assumption, considering an asymptotically slender turbulent shear layer. Amongst others, it is shown how a combination of a multiple-scales technique and matched asymptotic expansions leads to the internal splitting of the shear flow (having a large streamwise velocity deficit) that a has already been adopted successfully in former studies regarding its time-mean behaviour, by using rather conventional mixing length arguments.

GA/CTS4449/09: Miscellaneous.

Organiser: Patrick Jenny (ETH Zürich, Switzerland)
Co-organiser: Thomas Sattelmayer (TU München, Germany)

Active control of combustion instability using fuel-flow modulation. **Daniel Guyot** (TU Berlin, Germany), Christian Paschereit (TU Berlin, Germany) GA/CT3144/009

Modern gas turbine technology relies on lean premixed combustion to satisfy stringent governmental NOx emission restrictions. However, combustion systems operating in the lean premixed mode are highly susceptible to the excitation of high amplitude pressure and heat release fluctuations called thermoacoustic instability. These self-excited oscillations result from the interaction of unsteady heat release in the flame with the combustion chamber's acoustic field and usually lead to increased noise, reduced system performance and reduced system durability.

To minimise this drawback of lean premixed combustion and to ensure safe operation of the combustion system, active instability control can be applied. As described by Rayleigh's Criterion, self-excitation of a combustion system occurs if the fluctuations in heat release from the combustion process are in phase with the pressure fluctuations. Although the real instability processes are somewhat more complex, RayleighŠs Criterion pinpoints how dampening of thermoacoustic instability can be achieved. A common approach is to induce heat release fluctuations, which are out of phase with the pressure fluctuations. Modulated fuel injection is recognized to be an efficient active control method for attenuation of combustion instabilities.

In this work active control is applied to an atmospheric premix combustor test rig equipped with a swirl-stabilized burner by modulating the premix fuel flow. The employed control circuit incorporates condenser microphones recording the pressure oscillations inside the combustion chamber, and valves controlling the fuel mass flow into the combustion system. The microphone signals are processed and command signals are sent to the valves.

The results prove the control circuit's suitability for dampening thermoacoustic instability in a lean premix combustion system. Furthermore, modulation of premix fuel shows significantly lower NOx emissions in comparison to the more common approach of modulated (secondary) pilot fuel injection, as hot spots are avoided.

Generating turbulence using active grids. **Robert Stresing** (Universität Oldenburg, Germany), Joachim Peinke (Carl von Ossietzky Universität Oldenburg, Germany), Pascal Knebel (Carl von Ossietzky Universität Oldenburg, Germany), Mathias Hölzer (Universität Oldenburg, Germany) GA/CT4027/009

Stochastic analysis of turbulent flows generated in a wind tunnel by static grids show a rather large difference compared to the statistical properties found in atmospheric turbulent flows. It is problematic to create large-scale, high intensity turbulence with static grids that shows statistical properties similar to atmospheric turbulence. We present data from an active grid that was installed in the wind tunnel at the University of Oldenburg. The new active grid aims to allow us to generate large-scale homogeneous and quasi-isotropic turbulence. The resulting turbulent flow has a high intensity, a large integral length and shows a distribution similar to atmosperic turbulence.

The interaction of high-temperature heterogeneous jets with construction materials. **Eugene Maslov** (Tomsk Polytechnic University, Russian Federation) GA/CT900/009

High-temperature heterogeneous jets are used for perforation constructional material in power processing, as well as environmental and technical engineering. Analysis via mathematical modeling of this process is important in applied technology engineering. This mathematical model to describe interaction high temperature gases and particles with surface solid and stress–strain condition in mathematical include phase transition. This mathematical model to describe physical process for various values parameters high-temperature heterogeneous jet and physical and thermo-physical properties of material. The problem of accumulation on a still plate of a constructional at concurrence of a normal direction to a streamline surface to an axis of symmetry of a jet heterogeneous subsonic jet of a viscous liquid is solved. Results of the numerical a condition of interaction of solid particles with a surface of a plate are presented. The range of change of parameters of particles and jets at which a surface is established. The typical results of velocity field and temperature distribution which describe basic laws of researching process are represented. The temperature field is compared with experiment data and satisfaction agreement is shown.

Numerische Simulation der Verweilzeitverteilungen in Flotationszellen. **Mario Streng** (Universität Kassel, Germany), Olaf Wünsch (Universität Kassel, Germany) GA/CT2115/009

Verweilzeitverteilungen fluider und fester Partikel dienen zur Charakterisierung mechanischer Trennvorgänge in kontinuierlich durchströmten Apparaten. Die Verteilungen geben Auskunft darüber, wie lange die Partikel im Apparat verweilen. Je nach Prozeß sind breite oder schmale Verteilungsfunktionen erforderlich. Die numerische Simulation solcher Verweilzeitverteilungen auf Basis eines berechneten Strömungsfelds gelingt mit zwei unterschiedlichen Methoden. Zum einen durch die Berechnung vieler Bahnlinien, die den Apparat durchströmen und alle zur gleichen Zeit an verschiedenen Stellen des Eintrittsquerschnitts gestartet sind. Zum anderen über die Einführung einer zusätzlichen Variablen, die als Konzentration verstanden werden kann und deren Ausbreitung im Prozeßraum mittels einer Transportgleichung berechnet wird. Am Beispiel einer Flotationszelle (Rührapparat zur Trennung fester Partikel aus wässrigen Lösungen) werden die Verfahren in Abhängigkeit der Betriebsparameter miteinander verglichen. Der Einfluß der geometrischen Konfiguration von Einlaß und Auslaß auf die Verweilzeitsummenfunktionen wird gezeigt. Sind die Partikel leichter bzw. schwerer als das Fluid, ergeben sich Unterschiede im Vergleich zu masselosen Partikeln. Aus den Ergebnissen lassen sich Hinweise für die Optimierung solcher Prozesse bezüglich der Betriebsparameter entnehmen.

Density of critical points for Gaussian random functions. **Willi Möhring** (Max-Planck-Institut Göttingen, Germany), Horst Vogel (Universität Göttingen, Germany) GA/CT3061/009

Often turbulent phenomena are accompanied by random fluctuations of some scalar quantities. An important property of such salar functions are its critical points,especially their density and type. Letting exceptional cases aside one finds in two- and three-dimesional cases extrema and saddle points. It can be determined from the sign dstribution of the eigenvalues of the Hessian matrix of second derivatives of the function. For two-dimensional functions an easy application of the Poincare-index theorem shows that their densities of saddle points and extrema agree. It does not apply to three-dimensional functions. From Morse-theory one finds that the saddle point density cannot be smaller than the extrema density. Its actual value depends of course on the turbulent field.

Some indications on these quantities can be obtained from random matrix theory. Therefore we consider eigenvalue distributions of Gaussian random matrices. For scalar fields from homogeneous isotropic turbulence the matrices are taken from an orthogonal ensemble. Even if one assumes a Gaussian distribution of the matrices they are not taken from the well known Gaussian orthogonal ensemble (GOE) but from another ensemble which possesses also very interesting properties. For the ratio ρ of the density of saddle points to the density of extrema one obtains then

$$\rho = \frac{1057 + 348\sqrt{6}}{625} = 3.0551.$$

This value is only slightly above three, which would be obtained if one would assume an equidistribution of the eight different sign combinations.

GA/CTS4447/09: Combustion.

Organiser: Hannes Kröger (Universität Rostock, Germany)
Co-organiser: Thomas Sattelmayer (TU München, Germany)
Co-organiser: Patrick Jenny (ETH Zürich, Switzerland)

Extended flamelet model and improved interaction of chemistry and turbulence for modeling of partially-premixed combustion with a joint PDF method. **Michael Hegetschweiler** (ETH Zürich, Switzerland), Patrick Jenny (ETH Zürich, Switzerland) GA/CT2987/009

One of the main tasks in turbulent combustion modeling is to accurately describe turbulence reaction interaction. Here, a possible approach how to fulfill this in conjunction with a Joint Probability Density Function (JPDF) approach is shown. For non-premixed turbulent combustion without local extinction the laminar flamelet concept proved to be a good assumption. As a generalization of this approach for partially premixed combustion, an extendend flamelet model considering embedded laminar triple flames is described. From DNS data of e.g. lifted jet flames one knows that embedded edge flames establish at the fine scales. In our modeling approach such laminar triple flames are computed in isolation. At the inflow boundary, the mixture fraction Z varies linearly from zero to one and a constant velocity is applied, such that a steady flame gets stabilized within the domain. At the left and right boundaries, slip boundary conditions with $Z = 0$ and $Z = 1$ are applied. The scalar dissipation rate $\chi \sim 1/L^2$ can be adjusted by varying the width L of the domain. These precomputed tables are then mapped from the 2D physical space to a Z-τ-space, where τ is the residence time of a passive fluid particle in the flame convected along a streamline. In order to use the resulting tables for PDF simulations of turbulent partially premixed flames, mixture fraction $Z^*(t)$, scalar dissipation rate $\chi^*(t)$ and $\tau^*(t)$ have to modeled for each particle. Since reaction occurs only within a relatively small flammable Z-range, this 2D flamelet model is only applied if a particle is located in this range and otherwise a modified IEM mixing model is employed, to compute enthalpy and species mass fraction changes.

Note, that this model accounts for some of the major effects responsible for extinction and reignition in partially premixed turbulent flames.

Modeling of turbulent pre-mixed combustion with a joint PDF method. **Mathias Hack** (ETH Zürich, Switzerland), Patrick Jenny (ETH Zürich, Switzerland) GA/CT2676/009

In many combustion applications the flow field is highly turbulent, and therefore the numerical treatment of the interaction between turbulence and reaction is very crucial. A common model for premixed turbulent combustion is the one by Bray, Moss and Libby (BML). It was developed for simulations in the RANS context and assumes an infinitely thin flame. They introduced a progress variable $c \in \{0, 1\}$ to distinguish between burnt ($c = 1$) and unburnt ($c = 0$) gas. In addition, a transport equation for the Favre average of c, $\tilde{c}$, was derived, in which the turbulent transport and source terms have to be modeled.

Employing the same ideas in combination with a PDF method, where the progress variable c is transported by computational particles, leads to a consistent formulation with the $\tilde{c}$-equation in the BML approach. It is an advantage, however, that in the PDF equation the turbulent transport of c appears in closed form. Moreover, by introducing the burning time τ, the embedded quasi laminar 1D flame profile can be resolved. This is achieved by measuring the τ for each computational particle (the time since the particle's c-value switched from zero to one). Assuming that the flame front propagates with a known velocity s_L relative to the particle position, the evolution of the composition, including enthalpy, can be determined from precomputed tables, provided τ is known. The main challenge, which has to be addressed in this context, is to estimate the ignition probability (when does c switch from zero to one?). The modeling approach and possible closures for the source term are discussed and examined with numerical experiments.

Flame propagation in free vortices. **Hannes Kröger** (Universität Rostock, Germany), Nikolai Kornev (Universität Rostock, Germany), Egon Hassel (Universität Rostock, Germany), Detlef Wendig (Universität Rostock, Germany) GA/CT2293/009

Object of this paper are experimental and numerical investigations of the Combustion Induced Vortex Breakdown (CIVB) phenomenon in a free straight vortex. The experiments were performed using a swirl generation device. A swirling jet of premixed methane/air is ejected by this device into the ambient surrounding air. At some distance above the swirler nozzle, there is a ring burner mounted which holds a stationary flame. When conditions for a flashback are met, i.e. the swirl number exceeds S=0.25 at a equivalence ratio of ϕ=0.7, the flame of the ring burner propagates against the main flow back to the nozzle.

The isothermal flowfield has been studied experimentally under the flashback conditions (S=0.25) using Laser Doppler Velocimetry (LDV) and Particle Image Velocimetry (PIV). It follows from the measurements, that there is no vortex breakdown in the isothermal flow. Furthermore, the axial velocity in the isothermal flow exceed the turbulent burning velocity everywhere by a factor of at least two. Nevertheless, in the reacting flow with the same flow parameters, a flashback occurs. The flashback event was documented using high speed camera films.

To confirm experimental observations and gain more insight into the phenomenon, numerical simulations of the flashback event were performed using the open source finite volume code OpenFOAM. To model the influence of turbulence, the large-eddy simulation technique was applied. For combustion modelling, a flame surface wrinkling model was used.

LES simulations clearly show the appearance of a small area of negative axial velocities in front of the flame tip. This is a remarkable feature indicating the presence of the CIVB. Analysis of the LES data points out that the flame propagation against the main flow occurs mostly by induction effects caused by the circumferential vorticity appearing due to the radial expansion of the vortex tube. The expansion causes a strain field spiraling the vorticity field. On the contrary, the vorticity appearing due to the volume expansion caused by the combustion counteracts the flame flashback. The baroclinic effect promotes the flame propagation. However, its effect is small.

Mechanism of fire-tornado formation. **Yuri Rudi** (Tomsk State University, Russian Federation), Anatoly Grishin (Tomsk State University, Russian Federation) GA/CT903/009

Fire tornadoes refer to the kind of atmospheric tornados. As a rule, they are caused by the matt urban or forest fires. Mechanism of occurring and evolution in the tornado is impossible to investigate under the natural conditions. Therefore investigating a mechanism of the fire tornado formation is very important. Fire tornadoes were imitated under the laboratory conditions by means of three experimental set-ups based on twisting the ascending convective flow of the oil combustion products (modeling fires at the oil reservoirs), wooden constructions (modeling fires in the populated areas) and forest fuels (modeling forest fires). Convective flow was twisted by rotating the lower base of the substrate with forest fuels, rotating at the top fans of the ventilator and at the side by means of an air flow generated by aerodynamic pipe. All the fuels were placed on the special substrates. Then they were ignited. A diameter of the substrates in different tests amounted to (6, 7, 10, 12, 20)e-2 m, while the height was (2, 6, 12)e-2 m. The diameter of the substrates coincided with that of the combustion area. It is shown, that fire tornado formation does not depend on the method of their generation and the kinds of the forest fuels, but it is determined by the values of the density of the heat flow caused by combustion and by an angular velocity (frequency) of the cylinder rotation w=(1,1-1,3) Hz, in which the forest fuel is placed. When w />/ 1,3 Hz, the fire tornado was unstable and decomposed. Stable tornado occurs at the definite (critical) velocity of rotation, determined by equilibrium of the forces acting on the flame: providing a moment of twisting a vortex. The time of the stable combustion is 18-20 seconds. It was established, that in the flow twisted from the bottom the time of combustion was 10 percent less than without the flow twisting. It is explained by increasing the velocity of diffusion combustion at the expense of hydrogen supply from the environment, since in a radial direction an air from the environment arrives to column-shaped tornado, while a combustion regime in the tornado is diffusive. Hydrodynamic criteria of similarity of the problem to be solved Gr, Pr, Fr, Os have been estimated. Criterion dependencies between them have been found.

Interactions between compressibility and heat release in turbulent mixing layers. **Inga Mahle** (TU München, Germany), Rainer Friedrich (TU München, Germany) GA/CT994/009

When the convective Mach number increases, there is a large reduction in the thickness growth rate and the turbulent intensities of a mixing layer which has important implications for applications such as scramjet engines. Additionally, the damping effect of heat release due to combustion adds to the already stablizing effect of compressibility. Since perfect mixing of oxidizer and fuel is a pre-requisite for complete combustion, it is of particular interest to understand the mechanisms that play a role when compressibility and heat release interact.

With this aim, highly resolved DNS of inert and reacting temporally evolving mixing layers at different convective Mach numbers ($M_c = 0.15$, 0.7 and 1.1) are performed. All computations achieve a self-similar state with Reynolds numbers based on the instantaneous vorticity thickness between 10000 and 20000.

The present results show that besides a decrease of the production term in the balance equation of the streamwise Reynolds stress, the pressure-strain correlation in this equation is also reduced by both, compressibility and heat release. It can be shown that this is a consequence of the alterations

in the fluctuating pressure fields. Therefore, an investigation of the pressure fluctations leads to a further understanding of their changes by compressibility and heat release.

09, Posters

GA/PP896/009: **On aerodynamical optimization of wind-farm layout by genetic algorithm method.**

Presenter: Bosko Rasuo (University of Belgrade, Yugoslavia)
Co-author: Aleksandar Bengin (University of Belgrade, Yugoslavia)
Co-author: Aleksandar Veg (University of Belgrade, Yugoslavia)

This paper presents a method for determination of optimum positions of single wind turbines within the wind farms installed on arbitrary configured terrains, in order to achieve their maximum production effectiveness. This method is based on use of the genetic algorithm as optimization technique. The wind turbine aerodynamic calculation is unsteady, based on the blade modeled as a vortex lattice and a free-wake type airflow behind the blade. Optimization method is developed for two different fitness functions. Both functions use the total energy obtained from the farm as one of the key variables. The second also involves the total investments in a single wind turbine, so the optimization process can also include the total number of turbines as an additional variable. The method has been tested on several different terrain configurations, with special attention paid to the overall algorithm performance improvements by selecting certain genetic algorithm parameters.

10, Minisymposia

GA/MP29/010: Dynamics of transitional separation bubbles.

Organiser: Ulrich Rist (Universität Stuttgart, Germany)
Co-organiser: Stefan Braun (TU Wien, Austria)

Adverse pressure gradient laminar boundary layers at low to medium Reynolds numbers are strongly susceptible to separation. Due to the deceleration of the main flow the laminar boundary layer separates from the solid surface and typically undergoes fast laminar-turbulent transition which is followed by reattachment of the shear layer being already turbulent. The area of recirculating flow causing negative skin friction is called a *laminar separation bubble* (LSB) or alternatively a *transitional separation bubble*.

In general LSBs are known to affect the overall flow properties only minor but react very sensitively to external disturbances such as free-stream turbulence, impinging sound waves, structure vibrations etc., which may result in the *bursting* of the (short) bubble leading either to a more pronounced separated flow region or even global separation. Both cases are accompanied by sudden and often unwanted major changes of aerodynamic forces; e.g., loss of lift and increase of drag. It is mainly this fact which explains the undiminishing research interest in this phenomenon for more than seventy years which can be found in various applications: low Reynolds number aerodynamics, unmanned aerial vehicles, on the wings of man-carrying gliders, vanes of turbo-machines, blades of wind-energy converters, and even on the slats of large commercial jet-powered airliners.

Because of the complicated spatio-temporal flow structure of transitional separation bubbles the underlying flow physics is still not well understood. The idea of the present mini symposium is to give both an overview and a detailed look into particular problems associated with the emergence of LSBs, the transition process and its interference. Experts will present their most recent achievements in this attractive field of research using different approaches: stability theory, boundary layer asymptotics, direct numerical simulations, hot-wire measurements and particle-image velocimetry.

Experiments on control of laminar separation bubbles through passive and active techniques. **Alexander Dovgal** (Kristianovich Institute, Russian Federation), Victor Kozlov (Kristianovich Institute, Russian Federation) GA/MT439/010

Recent experimental data obtained in ITAM SB RAS on control of laminar separation bubbles at low subsonic velocities are summarized. In a low-turbulence wind tunnel, both passive and active control methods aimed at optimization of mean and oscillatory separated flow characteristics were examined. The methods employ stationary local and periodic modulations of a body surface, generation of acoustic waves, oscillatory and continuous suction of the near-wall fluid. A number of beneficial control effects have been observed through application of the above techniques. It is found that a promising way to improve operation of airfoils is utilization of a wavy lifting surface. In particular, modification of the separated flow pattern produced by the spanwise waviness of the wall prevents from global flow separation at high angles of attack increasing the critical incidence of airfoil. Also, the wind-tunnel data give indications of a strong response of separated flows on finite-span wings to 3D local stationary perturbations of the surface rearranging the entire flow pattern. Periodic forcing and suction applied to a back-step flow were found as effectively controlling the separated flow unsteadiness dominated by the large scale vortices shedding from the separation bubble. Thus, the energetic low frequency motion induced by separation bubbles can be suppressed. The above observations are discussed emphasizing fundamentals of the control approaches relevant to instability of laminar separating boundary layers.

3D vortical structures of a laminar separation bubble on an SD7003 airfoil. **Wolfgang Schroeder** (RWTH Aachen, Germany), Sebastian Burgmann (RWTH Aachen, Germany) GA/MT2346/010

The laminar separation bubble on the suction side of an SD7003 airfoil has been investigated using the Scanning Particle-Image Velocimetry (SPIV) technique. Due to an adverse pressure gradient the laminar boundary layer detaches at $Re_c < 100.000$. Transition occurs and leads to a turbulent reattachment of the separated shear layer enclosing a recirculation region. Kelvin-Helmholtz instabilities force the shear layer to roll up in the reattachment region such that vortices occur that separate from the main recirculation region and propagate downstream.
Using the Scanning PIV technique these vortical structures in the reattachment region can be analyzed in detail concerning the three-dimensional structure and their time-dependant development. For using the PIV technique the flow has to be seeded with small tracer particles. In an illuminated measurement plane the scattered light of the particles is detected with a camera. Recording the flow at least twice leads to particle images with a movement of the particles from picture 1 to 2. This particle movement can be converted into a velocity field using cross-correlation routines. The Scanning PIV technique uses a moving light-sheet to illuminate distinct planes within the measurement volume to investigate the flow field within a volume instead within a single plane. The separated flow of a SD7003 airfoil has been investigated at a Reynolds number of 20.000 and at angles of attack of $4°$ to $8°$. The size and position of the separation bubble has been analyzed as well as the flapping-frequency of the vortical structures that evolve in the reattachment region. Using a stereo set-up all three velocity components have been detected in each light-sheet plane leading to a quasi-three dimensional measurement of the reattachment region. Typical vortical structures like the c-shape vortex and the screwdriver vortex have been detected and their spatio-temporal development has been visualized.

3D effects on swept laminar separation bubbles. **Tilman Hetsch** (University of Southampton, UK), Ulrich Rist (Universität Stuttgart, Germany) GA/MT1418/010

Direct numerical simulation (DNS) is used as a tool to investigate different aspects of the influence of sweep on a series of pressure-induced laminar separation bubbles. So far research efforts have been nearly exclusively concentrated on unswept case. But in important technical applications, as on high lift devices of modern airliners, laminar separation bubbles appear naturally in swept geometries. Therefore, the talk concentrates on three phenomena connected with a swept inflow: 1. The effect of sweep on the undisturbed base flow itself. Based on the independence principle and backed by an experiment it can be shown that there is an universal topology of swept laminar separation bubbles in the geometry of an infinite swept wing. 2. The effect of different propagation directions of the primary disturbance in fundamental transition scenarios on the onset of transition. It turns out that two-dimensional Tollmien-Schlichting waves, which are so important in the unswept case, quickly loose their dominance to oblique TS-waves as the sweep angle increases. 3. The growing influence of cross-flow instabilities with rising sweep angle. The interaction of high-amplitude stationary crossflow vortices on the fundamental transition scenarios investigated before is studied for the high sweep angle of 45 degrees.

Mean flow deformation in a laminar separation bubble. **Olaf Marxen** (Stanford University, USA), Ulrich Rist (Universität Stuttgart, Germany) GA/MT887/010

An important effect occurring during laminar-turbulent transition in a pressure-induced laminar separation bubble on a flat plate is investigated by means of Direct Numerical Simulations. Such a separation bubble can originate if a boundary layer is subject to a sufficiently-strong adverse pressure gradient. Transition occurs in the detached shear-layer, which in most cases results in mean reattachment, thus forming a closed bubble in the mean.

The investigation of the effect of mean flow deformation (MFD) is devoted to the upstream; i.e., feedback, effect on the flow in the mean, caused by a small, unsteady disturbance input that provokes transition. With such a disturbance, the resulting viscous-inviscid interaction evokes a large mean flow deformation; i.e., a change of the flow field in the mean, that reaches far upstream. While the MFD at transition is caused directly via the non-linearity of the Navier–Stokes equations, the mean flow deformation upstream is induced indirectly via a change in the streamwise pressure distribution caused by the saturated disturbances. It is shown that the effect of this mean flow deformation in the potential-flow region further away from the wall can be modeled using a source/sink distribution at the wall.

Two different central effects are observed that are caused by the small disturbance input: a reduction of the size of the separation region (i.e., a smaller separation bubble in the mean); and a stabilization of the flow with respect to small, linear perturbations upstream (i.e., in the laminar part). Aided by the application of linear stability theory it is shown that studies of linear perturbations in disturbance formulation are meaningful if based on the deformed, time-averaged flow field only; i.e., for a known transition process.

GA/MP29/010: Dynamics of transitional separation bubbles. #2

Organiser: Ulrich Rist (Universität Stuttgart, Germany)
Co-organiser: Stefan Braun (TU Wien, Austria)

(For abstract, see session #1 above.)

Transitional separation bubbles on airfoils. **Neil Sandham** (University of Southampton, UK), Lloyd Jones (University of Southampton, UK) GA/MT2700/010

An unsteady viscous-inviscid interaction method is tested against recent results from direct numerical simulation and experiment. The unsteady method is a time-accurate extension of traditional methods of coupling integral boundary-layer methods with a potential flow solution based on panel methods. The unsteady formulation, including an envelope-based transition model is shown to be capable of predicting large-amplitude low-Strouhal number oscillations as seen in several recent experiments. Above a critical incidence the airfoil separation bubble reattachment point can no longer be held and the flow develops a limit cycle behaviour in which the bubble growth leads to fully stalled flow followed by a reformation of the bubble. The mechanism depends on strong coupling between the potential flow and the boundary layer. The unsteady model is also calibrated against results from recent direct numerical simulations of separation bubbles on NACA-0012 airfoils. At low incidences the airfoils exhibit short separation bubbles with convective growth of instabilities. At higher incidence we investigate the simulation and modelling of airfoils with localized regions of absolute instability.

DNS of laminar separation bubble flows with free-stream fluctuations. **Jan Wissink** (Universität Karlsruhe, Germany), Wolfgang Rodi (Universität Karlsruhe, Germany) GA/MT1302/010

In the presence of a strong enough adverse pressure gradient, a laminar boundary layer over a flat plate will separate. The separated boundary layer (shear layer) is very unstable and will usually undergo rapid transition to turbulence. Experiments showed that the presence of external fluctuations can drastically reduce the size of a Laminar Separation Bubble (LSB). To elucidate the physical mechanisms involved, a series of Direct Numerical Simulations (DNS) of separating boundary-layer flows over a flat plate were performed.

In accordance with the companion experiments performed at the Technical University of Berlin, in the DNS the adverse pressure gradient was induced by a contoured upper wall. In the spanwise direction of the computational domain periodic boundary conditions were employed, while at the outlet a convective outflow condition was prescribed. The Reynolds number of the flow problem, based on the local free-stream velocity and the momentum loss thickness, θ, of the boundary layer just before separation was approximately $\mathrm{Re}_\theta = 90$.

The influence of two types of free-stream fluctuations, both superposed on a uniform inflow, on the dynamics of the LSB were considered:

1. A streamwise oscillation of which both the amplitude and the period were varied
2. Grid *turbulence* of which the level was varied

In all simulations, the primary mechanism for the transition to turbulence was found to be a two-dimensional Kelvin–Helmholtz (KH) instability of the separated shear layer that was triggered by the external fluctuation(s). The KH instability caused the shear layer to roll up. Inside the rolled up shear layer, entrained disturbances triggered elliptic instabilities which led to a rapid transition to fully three-dimensional (3D) turbulence.

Global stability calculations of separated flows. **Jitesh Gajjar** (University of Manchester, UK) GA/MT1562/010

The primary motivation for the current work is to develop suitable techniques for studying the global instability in many different flows such as that occuring in the flow past a row of circular cylinders placed in a uniform stream, see Gajjar & Azzam (2005), or in the supersonic flow past a compression ramp, Fletcher et.al. (2004). In the latter problem, for sufficiently large ramp angles, the flow in the recirculation region near the corner becomes unstable and it was suggested in Fletcher et.al. (2004) that an absolute instability may be responsible for the abrupt local breakdown of the bounday layer. In both these quite different problems a common difficulty is the generation of the mean steady flow which is needed for input into an eigenvalue solver. For the flow past a circular cylinder, the accurate computation of the steady flow is difficult, as the work of Gajjar & Azzam (2005) and Fornberg (1991) has demonstrated. The precise manner in which the equations and boundary conditions are handled, and the accuracy of the numerical techniques used is very important, and crude techniques do not work well. In the supersonic corner ramp problem, the computations of the steady flow encounter severe difficulty especially for large corner angles when secondary separation is present, see Korolev et. al. (2002). Here, even with

sophisticated numerical methods, large-scale separation poses considerable problems.

In the current work we have extended the methods used to compute the steady flow past a cascade of circular cylinders, and the supersonic flow past a compression ramp, to study the global instability of these flows. In this talk we will discuss the methodology and the results obtained.

Convective and global instabilities in separated flows. **Jean-Christophe Robinet** (École Nationale Supérieure d'Arts et Métiers, France) GA/MT1103/010

The following paper is devoted to laminar separated boundary-layer flows of incompressible fluids. Laminar boundary-layer separation is a fondamental phenomenon and has a number of related applications. Low Reynolds number aerodynamics of airfoils, flow over steps, humps and other kinds of localized variations of a surface are striking examples of aerodynamical problem which concern laminar separation. Thus, laminar separated flows have been addressed for decades and significant success has been achieved in experimental, numerical and theoretical studies.

A feature of laminar separated flows is that they become unstable even at relatively low Reynolds numbers. As a result, such flows usually involve unsteadiness and a transition to turbulence. In the most of cases, when considering the evolution of oscillations in a separated flow, the primary instability is assumed to be convective. Nevertheless, an absolute instability can occur in the strong back-flow regimes (Rist & Maucher, 2002).

More recently Theofilis *et al.* (2000) have shown that there is a three-dimensional and stationary instability wave family not envisaged by the weakly non-parallel theories being able to play an important part in the transition mechanisms. However,this study does not consider the case where there are at the same time convectives instabilities coming from the upstream of the flow and an intrinsic global instability in the separated zone. The objective of this paper is to show that a global stability approach of a laminar separated flow permits to study the case where the flow is at the same time convectively unstable at upstream and downstream to the separated zone and globally unstable in separated zone. Two families of modes will be shown: spatially convective global modes and non convective global modes.

GA/MP29/010: Dynamics of transitional separation bubbles. #3

Organiser: Ulrich Rist (Universität Stuttgart, Germany)
Co-organiser: Stefan Braun (TU Wien, Austria)

(For abstract, see session #1 above.)

Laminar separation bubbles from a high Reynolds-number asymptotic point of view. **Stefan Braun** (TU Wien, Austria) GA/MT1943/010

Classical boundary layer theory proved to lose its validity if flow separation is encountered. However, introduction of the triple deck concept – i.e. allowing for the displacement effect of the viscous boundary layer to interact locally with the induced pressure (disturbances) in the outer inviscid flow regime – led to a successful description of 'short' laminar separation bubbles in various fundamental flow problems. Here we want to focus on situations which share the following distinctive feature: two-dimensional steady state solutions of the underlying interaction equations exist in a limited range of values of a parameter controlling the conditions leading to separation only. Furthermore, these solutions turn out to be non-unique in the vicinity of the limiting *critical* value of this parameter. Typical examples include leading edge separation, smooth backward facing step flow, channel flow with suction, subsonic expansion ramp flow, asymmetric trailing edge separation etc. More recent investigations which take into account (local) unsteady, three-dimensional and flow control device effects and concentrate on *near critical* flows indicate that *(i)* exceeding the critical value of the controlling parameter is associated with self-sustained vortex shedding (time periodic bubble 'bursting' even in the absence of external disturbances), *(ii)* coherent structure formation caused by bubble bursting events turns out to be essentially self-similar, *(iii)* the high sensitivity of the separated flow region with respect to external disturbances allows for effective application of (optimized) flow control devices in order to force or delay the transition process to turbulent boundary layer flow. The aim of the presentation is to deliver insight into the achievements of modern asymptotic analysis in the topic under consideration.

On viscous–inviscid interaction in transonic flows. **Anatoly Ruban** (University of Manchester, UK) GA/MT2211/010

This paper is concerned with theoretical analysis of the behaviour of the transonic flow past a convex corner on a rigid body surface. It is known from experiment that the flow can take two forms, with separation from the corner and attached form of the flow. The latter undergoes fast acceleration from subsonic speed before the corner to supersonic Prandtl-Meyer flow behind the corner.

Assuming the Reynolds number large, we starts with the inviscid part of the flow, where the solution of the Kármán-Guderley equation may be constructed analytically using the hodograph method. This gives the pressure distribution for the boundary layer that forms on the body surface. The pressure gradient appears to be different for the separated and attached flow regimes. However, in both cases a singularity develops on approach to the corner; for the separated flow $dp/dx \sim (-x)^{-1/3}$, while for the attached flow $dp/dx \sim (-x)^{-3/5}$. Here p denote the pressure and x the distance from the corner apex.

The solution for the boundary layer also develops a singularity. It splits up into two parts, viscous near-wall sublayer and locally inviscid main part of the boundary layer. We found that contrary to what happens in subsonic and supersonic flows, the contribution of the main part of the boundary layer contributes into the displacement effect is no longer negligible. In fact, for the separated flow regime it dominates the contribution of the viscous sublayer. For the attached flow, the two parts of the boundary layer contribute equally. However, in this case, an intermediate layer forms between viscous and inviscid parts of the boundary, and this is the intermediate layer that defines the displacement effect of the boundary layer as a whole.

The presentation will be concluded with the discussion of the solutions for the viscous-inviscid interaction region that forms near the corner.

Receptivity of the boundary layer with separation bubble to external sound waves. **Vladimir Zametaev** (Central Aerohydrodynamic Institute, Russian Federation), Marina Kravtsova (Central Aerohydrodynamic Institute, Russian Federation) GA/MT2309/010

The receptivity problem of laminar separated two-dimensional boundary-layer under influence of external acoustic waves is considered. Basic features of this theory were formulated by Ruban (1984) and Goldstein (1985), but these investigations were limited by small perturbations of steady parallel flow only. This paper is concerned with essentially nonparallel regimes of base flow, including attached flows, flow with separated bubbles and base flow at marginal value of the main parameter. The steady flow near a corner point of profile is of considerable interest and a question naturally arises about the sensitivity of separation bubble inside the BL to external disturbances such as sound waves. Another question arises about the sensitivity of near critical base flow, namely if corner is convex there is a marginal angle which limits existence of such base interaction flow. This fact usually is linked with a sudden reconstruction of full flow pattern past a profile. Development of perturbations inside the interaction region may give some answers on the T-S waves development and appearance of turbulence. The asymptotic problem includes two set of equations. The first boundary-layer problem describes the separation flow near a corner point of a rigid body contour. The steady solution is calculated using an effective numerical method. Second unsteady interaction problem describes development of periodical in time perturbations incoming from upstream. Calculations were made for different regimes including attached and separated flows. First of all for zero displacement to study development and viscous decreasing of perturbations for different values of the frequency of sound wave ω and then taking into account interaction process. It is of interest that perturbation which achieves zone of separation has fast periodical behavior with large amplitude. Full problem calculations were made and results describe sharp development of perturbation along the interaction region. /enddocument

Dynamical flow phenomena associated with the laminar separation bubble on an SD7003 airfoil. **Christian Kaehler** (TU Braunschweig, Germany), Rainer Hain (TU Braunschweig, Germany) IC/MT4439/010

In the past, many numerical and experimental investigations on Laminar Separation Bubbles (LSB) have been performed, see Lang et al. (2001) and Radespiel et al. (2006) for instance. One reason is that these bubbles can have a strong influence on the flow around an airfoil so that both the lift and the drag are affected. The LSB's mainly occur at thin airfoils at Reynolds numbers $Re = 5 \times 10^4$ - 5×10^5. Many of the investigations of LSB's were done for generic test cases or by means of measurement techniques which do not allow capturing the flow phenomena with a high spatial and temporal resolution (e.g. LDA or conventional PIV). Ol et al. (2005) summarizes a comparison between investigations on the SD7003 airfoil at Re = 60000 and an angle of attack of 4° in different test facilities. The measurements were done by means of conventional PIV to determine statistical quantities such as the size and shape of the bubble, the onset of turbulence in the shear layer and the point of were the turbulent reattachment takes place.

To understand the complex 3D flow topology of the laminar separation bubble with the transition and vortex shedding process, the temporal evolution of the flow structures was investigated by Hain et al. (2005) with different time resolved PIV techniques. Beside the 3D topology the dominant frequencies of the transition process and the vortex shedding were determined. In order to investigate the dynamic processes in further detail, scanning PIV measurements have been performed on a SD7003 airfoil at a Reynolds number of Re = 60000.

Different light sheet orientations were realized in order to analyse the three-dimensional dynamic of the shed vortices. In the configuration with the light sheet parallel to the airfoil surface, the interaction between the vortices can clearly be seen. The light sheet orientation normal to the airfoil in main flow direction allows a detailed analysis of the transition process. Based on these experiments a detailed understanding of the dynamical processes could be established as will be outlined at the conference.Lang M, Marxen O, Rist U, Wagner S: Experimental and numerical investigations on transition in a laminar separation bubble. In: S. Wagner, U. Rist, H.J. Heinemann, R. Hilbig (eds.): New Results in Numerical and Experimental Fluid Mechanics III, Proc. 12. DGLR-Fachsymposium AG STAB, Stuttgart, 15.-17.11.2000, NNFM Vol. 77, Springer Verlag, 2001Radespiel R, Windte J, Scholz U: Numerical and Experimental Flow Analysis of Moving Airfoils with Laminar Separation Bubbles. AIAA-2006-0501, 2006Ol MV, McAuliffe BR, Hanff ES, Scholz U, Kaehler CJ: Comparison of laminar separation bubble measurements on a low Reynolds number airfoil in three facilities, AIAA-2005-5149, 35th AIAA Fluid Dynamics Conference and Exhibit, Toronto, Ontario, June 6-9, 2005 Hain R, Kaehler CJ: Advanced Evaluation of Time-Resolved PIV Image Sequences. 6th International Symposium on Particle Image, Pasadena, California, September 21-23, 2005

GA/MP142/010: Influence of the geometry of the boundary on flows in layers.

Organiser: Markus Scholle (Universität Bayreuth, Germany)
Co-organiser: Hannes Uecker (Universität Stuttgart, Germany)

Fluid layers frequently occur in nature as well as in technology. Rain wetted roads or the tear film of the eye are examples for films encountered in environmental or biological systems. In industries, we find fluid layers in coating applications and lubrication problems. In the past, much attention was paid to the stability of plane films, whereas in recent times the influence of the wall topography due to e.g. steps, trenches or periodic corrugations on the flow has become subject of detailed investigations, increasingly. These investigations deliver creation of kinematically induced eddies in creeping flows, a shift of the stability limit in flows at moderate Reynolds numbers and pattern formation like hydraulic jumps and nonlinear resonance effects at higher Reynolds numbers. Consequences for material and heat transport induced by eddies are also subject of this minisymposium.

Stationary solutions and linear stability for film flow over wavy bottoms for large Reynolds numbers. **Tobias Häcker** (Universität Stuttgart, Germany) GA/MT4468/010

We study the flow of an incompressible liquid down an incline with a periodically undulated bottom. In the case of high Reynolds numbers we derive an Integral Boundary Layer equation as a thin film approximation. This has spatially steady solutions which can be expanded in terms of the dimensionless film thickness. With a linear stability analysis based on Bloch wave transformation we show the existence of a critical Reynolds number corresponding to the results over flat inclines.

Inertial effects in film flow along strongly deformed walls: deep periodic corrugations and abrupt steps. **Vasilis Bontozoglou** (University of Thessaly, Greece) GA/MT558/010

Liquid film flows are of central importance in many industrial processes. The wall on which the film moves is frequently irregular, either intensionally as in process intensification or accidentally as in the coating of defective surfaces. This talk presents recent computational findings on the free surface configurations and flow structures attained along strongly deformed walls.

A periodically corrugated wall is known to resonate with the liquid film, resulting in a steady flow with strongly deformed free surface. Deep corrugations eventually lead to steady separation, whose extent at $\mathrm{Re} = O(10)$ depends non-monotonically on film thickness. For thick films the separation region tends asymptotically to cover half of the corrugation trough and the resulting flow structure has similarities with creeping flow. For progressively thinner films, the separation region initially shrinks (or even disappears) but then grows impressively to cover most of the corrugation trough. The latter behavior is attributed to the combined effect of the strong wall and free surface deformations, whose phase difference induces a pinching of the film that triggers inertial separation.

Isolated orthogonal steps along an otherwise flat wall induce local deformations (ridges, depressions) on the upstream side of the free surface, which provide the capillary pressure needed to change the flow direction. The characteristic length of these deformations is predicted from simple scaling arguments, and the transition from a capillary-gravity to a capillary-inertia regime is identified. With increasing Re, the upstream deformations initially intensify but subsequently receed and disappear. This change is understood as a result of increasing flow separation, which smoothens the directional variations induced by topography. At higher Re, purely inertial deformations appear, which are produced by liquid overshoot at the exit of the step. Here, capillarity is resisting deformation, and thus the dependence on surface tension is reversed.

Resonance in viscous film flow over topography. **Andreas Wierschem** (TU München, Germany), Vasilis Bontozoglou (University of Thessaly, Greece), Christian Heining (Universität Bayreuth, Germany), Nuri Aksel (Universität Bayreuth, Germany) GA/MT1159/010

We study viscous gravity-driven films flowing over periodically undulated substrates numerically, analytically, and experimentally. Linear analysis describes resonance in steady flow along small amplitude corrugations for films of arbitrary thickness. Depending on the dimensionless film thickness we find different regimes for the resonance, which is associated with the interaction of the undulated film with capillary-gravity waves traveling against the flow. Nonlinear resonance produces higher harmonics and bistable resonance. The higher harmonics are due to higher-harmonics resonance and due to the nonlinear coupling to lower harmonics. For the bistable resonance we derive a minimum model showing that the bistability corresponds essentially to that of the driven Duffing oscillator.

Nonlinear stability for film flow over wavy bottom. **Hannes Uecker** (Universität Stuttgart, Germany) GA/MT1082/010

We consider a spatially periodic Kuramoto–Sivashinsky equation as a model problem for inclined film flow over wavy bottoms and other spatially periodic systems with a long wave instability. We show that linearly stable stationary solutions are also nonlinearly stable, and that perturbations decay in a characteristic self similar way determined by a Burgers equation in Bloch wave space, which is the amplitude equation of the problem.

The analysis is based on Bloch wave transform and renormalization group methods.

GA/MP142/010: Influence of the geometry of the boundary on flows in layers. #2

Organiser: Markus Scholle (Universität Bayreuth, Germany)
Co-organiser: Hannes Uecker (Universität Stuttgart, Germany)

(For abstract, see session #1 above.)

Numerical simulation for the flow of continuous thin liquid films over topography. **Harvey Thompson** (University of Leeds, UK), Philip Gaskell (University of Leeds, UK), Yeaw Chu Lee (University of Leeds, UK), Markus Scholle (Universität Bayreuth, Germany), Nuri Aksel (Universität Bayreuth, Germany) GA/MT1111/010

Free surface full film flows over topography are of great scientific interest and play a vital role in several important biological, engineering and manufacturing processes. However, the unravelling of such flows presents a considerable challenge to experimentalists and theoreticians alike; the investigation of the effects of localised topography being particularly demanding. Accordingly, this paper considers the present state-of-the-art associated with the accurate numerical solution of such problems for a range of three-dimensional flows.

The benefits of employing a lubrication framework to derive a tractable set of governing equations for Stokes' flow, with their resulting Finite Volume analogues solved optimally using an implicit multigrid scheme, is demonstrated. Reported also are the benefits to be accrued from implementing automatic error-balanced mesh adaptivity and time integration without loss of accuracy.

Solutions to a number of three-dimensional gravity-driven flow problems are presented, which include: (i) continuous thin film flows over single and grouped topography; (ii) the effects of evaporation for the same; (iii) the presence of occlusions (blockages) in regions of the flow domain; (iv) minimisation of free-surface disturbances.

Finally, from the point of view of establishing the appropriateness or otherwise of pushing the bounds of the lubrication approximation to solve the above problems, the importance of inertia is quantified by comparing solutions obtained for the simpler case of flow over two-dimensional topography; with corresponding results obtained using a finite element discretisation of the associated Navier-Stokes equations

Influence of eddies on heat transfer in Couette flow over undulated substrates. **Markus Scholle** (Universität Bayreuth, Germany), Harvey Thompson (University of Leeds, UK), Nuri Aksel (Universität Bayreuth, Germany), Philip Gaskell (University of Leeds, UK) GA/MT1036/010

In Couette flows over undulated substrates eddies can be generated under creeping flow conditions. In contrast to free surface flows on undulated substrates even smooth bottom undulations allow for eddy generation due to the kinematical constraints. The subject of our paper is how these flow patterns interact with the temperature field in non-isothermal flows.

We consider the steady Couette flow of a Newtonian fluid between two plates, one of them planar, the other one with a sinusoidal profile. Additionally, a transversal heat flux is imposed by a temperature difference between the two plates. Our analysis of the thermo-mechanical coupling is focused on the two dominant effects, namely convection and thermoviscosity, whereas dissipation heat, buoyancy and temperature-dependence of the remaining material parameters are neglected.

We solve the problem in two steps: First, the influence of the eddies on the convective heat transfer is considered by solving the heat conduction equation with convection. For the velocity field we take the solution resulting analytically from Reynolds' lubrication approximation for the isothermal flow. Second, the thermoviscous feedback of the resulting temperature field to the flow is taken into account.

For the construction of the solution an analytical approach based on a non–orthogonal series representation of the fundamental fields and a variational formulation of the field equations is used. The results are visualised and the physical effects they reveal are discussed.

10, Short Communications

GA/CTS4875/10: **Rheology and multiphase flows.**

Organiser: Guenter Brenn (TU Graz, Austria)
Co-organiser: Ewald Krämer (Universität Stuttgart, Germany)

Numerische Strömungssimulation viskoelastischer Fluide . **Olaf Wünsch** (Universität Kassel, Germany), Mathias Krebs (Universität Kassel, Germany) GA/CT2162/010

Bei der Simulation von Strömungen von Flüssigkeiten mit Gedächtnis müssen die aktuellen Reibungsspannungen aus der Geschichte der relativen Deformationen berechnet werden. Dies kann einerseits mit integralen Materialmodellen erfolgen, erfordert aber die Verfolgung der Fluidelemente auf ihren Bahnen in die Vergangenheit und die Integration der dabei erlebten Deformationen. Dagegen werden bei den differentiellen Modellen nur die Spannungen und Deformationen zur aktuellen Zeit benötigt, allerdings auch deren zeitliche Ableitungen. Letztere Modelle führen bei der Strömungsberechnung auf zusätzliche Differentialgleichungen für die Spannungskomponenten, die simultan mit den Bewegungsgleichungen und der Kontinuitätsgleichung gelöst werden müssen. In diesem Vortrag geht es um numerische Berechnungen von Strömungen mit differentiellen Stoffmodellen unter Verwendung eines finiten Volumenverfahrens. Die zusätzlichen Spannungsdifferentialgleichungen lassen sich in Form von Transportgleichungen in das Verfahren integrieren. Beim Lösen der Gleichungen muss auf deren speziellen numerischen Eigenschaften Rücksicht genommen werden. Verschiedene Materialmodelle (Oldroyd, Giesekus, Tanner) kommen zum Einsatz, deren Eignung zur Beschreibung realer, hochviskoser Füssigkeiten diskutiert werden. An Hand von Strömungsimulationen in zweidimensionalen Geometrien wird die Vorgehensweise bei der Berechnung gezeigt. Die Ergebnisse werden mit analytischen Berechnungen und Literaturdaten verglichen. Schließlich erfolgt die Anwendung des Verfahrens auf Strömungen in realen, dreidimensionalen Geometrien. Bei der Umströmung von Partikeln und der Durchströmung von Apparaten der Verfahrenstechnik sind deutliche Einflüsse der Viskoelastizität zu erkennen.

Simulation der anisothermen Strömung in einem Doppelschneckenextruder. **Carsten Conzen** (Universität Kassel, Germany), Olaf Wünsch (Universität Kassel, Germany) GA/CT2118/010

Doppelschneckenextruder werden im Maschinenbau und in der Verfahrenstechnik zur Förderung und Homogenisierung von hochviskosen Flüssigkeiten, wie z.B. Kunststoffschmelzen verwendet. Experimente und numerische Berechnungen zeigen, dass bei schleichenden Strömungen hochvikoser Fluide mit geringer thermischer Leitfähigkeit $(Re \to 0, Pe \geq 10^4)$ die Entwicklung des Strömungs- und des Temperaturfeldes auf verschiedenen Orts- und Zeitskalen stattfindet. Zudem wird aufgrund der hohen Viskosität die zur Förderung notwendige mechanische Energie zu einem großen Teil im Fluid dissipiert. In Kombination mit der geringen Wärmeleitfähigkeit führt dies zur Ausbildung eines inhomogenen und instationären Temperaturfeldes in der Flüssigkeit. So kann es passieren, dass die Kunststoffschmelze in Extrudern lokal so stark erhitzt wird, dass die physikalischen Eigenschaften des Materials sich irreversibel verändern. Dieser Vortrag stellt die Vorgehensweise und die Ergebnisse der numerischen Strömungs- und Temperaturfeldberechnung in einem Doppelschneckenextruder vor. Dazu werden dynamische d.h. zeitlich veränderliche Netze verwendet. Das strukturviskose Verhalten sowie die Temperaturabhängigkeit der Viskosität des Fluids fließen in die Berechnung ein. Die gewonnenen Ergebnisse in Abhängigkeit der Betriebsparameter werden diskutiert und mit experimentellen Daten einer Modellflüssigkeit verglichen.

Experimental validation of a visco-elastic material model for numerical simulation of the extrusion process of rubber blends. **Herbert Müllner** (TU Wien, Austria), André Wieczorek (TU Wien, Austria), Pia Petracek (TU Wien, Austria), Josef Eberhardsteiner (TU Wien, Austria) GA/CT1923/010

The dimensioning of injection heads for the extrusion of rubber profiles is exclusively based on empiric knowledge of the non-linear viscoelastic flow behavior of elastomers. Thus, the design of injection heads is carried out with subject to the used rubber blend, whereas the geometry of the appropriate profile is achieved by empiric adaptation of the extrusion die. The non-reproducible process technology affects the capacity of the running production relevantly. This work was performed in cooperation with Semperit Technische Produkte GmbH, which provided the rubber blends as well as the experimental devices.

An important task of a constitutive material characterization is the determination of a viscosity function, which can be used for arbitrary parts of instruments for the production of rubber profiles. Till now, capillary-rheometry is the most important method for the determination of the viscosity of common rubber compounds as well as rubber blends. Due to application problems for the investigated rubber blends, new concepts were developed for the identification of its viscoelastic properties without using correction methods [1].

From numerical simulations with variable power law constants material independent diagrams are obtained. For the validation of the new parameter identification a comparison between performed measurements and the numerical simulations of the corresponding situation is chosen. The simulations have been performed with the commercial CFD program POLYFLOW.

Therefore, all important state variables have been discussed, as experimental quantities like melt pressure and die swell measurements. The experimental validation of various capillary experiments shows good agreement between the results of the characterization methods [1] and the numerical simulations.

[1] H.W. Müllner, J. Eberhardsteiner, K. Hofstetter: Viscosity Characterization for Rubber Blends from Die Swell Data by Means of Genetic Algorithms. PAMM, Vol. 6 (2006): accepted.

Drop deformation under surfactants adsorbtion. **Ioan-Raducan Stan** (Universitatea Babeş-Bolyai, Romania), Maria Tomoaia-Cotisel (Universitatea Babeş-Bolyai, Romania), Aurelia Stan (Cluj-Napoca, Romania) GA/CT3257/010

The movements of free liquid drops resulting from unbalanced surface tension gradients constitute important surface phenomena (Marangoni effect). It is well-known that a free liquid drop, submerged in an immiscible liquid undergoes complicate motions, when an interfacial tension gradient arises on their surface (in our case the adsorbtion of a surfactant). So linear and rotational displacements of the drop, oscillations, surface waves, deformations (even fission), have been experimentally evidenced. Theirs study is of present interest in the mass transfer processes, in conceiving models of movement at the biological membrane level, as well as in the space science and technology of liquids.

The aim of this paper is to correlate the effect of pressure forces on the drop, with the surface coverage degree, namely on the extent to which the drop surface is covered with surfactant. Our model show that for a covered degree less then 680, these forces are negative, this means that the force exerted by the external liquid upon the drop is oriented towards the negative direction of the normal to the drop surface, acting like a hammer.

We consider that is a direct connection between this force and the deformation of the drop. We showed that at small values of this force the drop remain undeformable, while for large values of force deformations and even fission of the drop may appears. However, there is more mechanism through which surfactants change the drop deformation. We mention here surface dilution, tip- stretching and capillary forces, but they appears as o consequence of the increase of the surface area of the drop when it is deformed to a nonspherical shape by the hammer force. The existence of this hammer force caused by the adsorbtion of a surfactant is in good agreement with our experimental data for different tension gradients and viscosities.

Linearized description of the flow of a vapor with condensation and evaporation through a micro-porous membrane. **Thomas Loimer** (TU Wien, Austria) GA/CT2701/010

The one-dimensional flow of a fluid near saturation through a micro-porous membrane is considered. Upstream of the porous membrane the fluid is in a state of saturated vapor. Downstream, the fluid is in a state of unsaturated vapor. Due to the Joule-Thomson effect, the fluid is cooler at the downstream side of the membrane than at the upstream side. Due to the temperature difference and the heat conduction in downstream direction, the saturated vapor condenses fully or partially and the fluid re-evaporates further downstream. The flow process is described taking into account (i) the temperature difference due to the Joule-Thomson effect, (ii) the capillary pressure across curved menisci in the porous medium and (iii) the vapor pressure reduction at curved menisci given by Kelvin's equation. Depending on the material properties of the fluid and the membrane and on the pressure difference, nine different types of flow occur. These types of flow are distinguished by the location of the condensation and evaporation fronts and whether the fluid condenses fully or partially. The different flow types are presented and a map is drawn to show the conditions under which they occur. The mass flux through the porous membrane is calculated and a comparison is made with experimental data.

Mathematical modelling of impregnation process. **Iryna Tkachenko** (Dnipropetrovs'k National University, Ukraine) GA/CT3806/010

Impregnation processes are an important part of many modern technologies dealing with porous media. As a rule the ŞdryŤ and ŞwettedŤ parts of porous body are separates by narrow domain which is called impregnation front or impregnation boundary and assumed asymptotically thin. Thus the impregnation process is described by moving boundary problem. Let us assume that the porous media in the considered problem is homogeneous and saturated in the ŞwettedŤ part, the impregnating liquid is incompressible, Darcy low takes place for filtration flow and then the filtration flow is described by Laplace equation with respect to pressure. The caution of the impregnation process is so-called wetting force that is capillary effect, which creates a pressure jump (called capillary height) on the impregnation front. At the first stage of the investigation a problem about the impregnation of spherical and cylindrical bodies which were instantly submerged into the liquid was considered. It is supposed that the impregnation process is regular. This assumption excludes from consideration an initial stage of impregnation process. The gas domain remains inside the body during the process. This domain is filled by the gas, which was in the body before the submerging. The process of impregnation continues until the gas pressure has become equal to the liquid pressure plus capillary height. In the considered case the pressure changes only along the bodyŠs radius. Then the boundary-value problem for Laplace equation is reduced to boundary-value problem for second order ordinary differential equation. Beside of that, Cauchy problem must be formulated to describe a motion of impregnation front. The analytical solutions for both cases are obtained. The next stage of the present work is solution of the same problems but in two-dimensional and three-dimensional formulation. Cartesian coordinates system is used in these cases. An analytical solution of two- and three-dimensional problems is very difficult and really possible for only very restricted number of cases. That is why the problems must be analyzed by some numerical method. It is well-known that the boundary element method is especially effective for elliptical boundary-value problems with linear differential operator, because the process of numerical solution is localized on the boundary alone. More than that, if there is a non-linear boundary condition, it gives additional advantages to boundary element method in comparison with other numerical methods. Zero order boundary element method is used in the present work. The considered above examples of analytical solutions are used as test problems during algorithm and computer code development. The proposed approach is illustrated by several examples of numerical calculations.

GA/CTS4879/10: Aerodynamics and fuel sloshing.

Organiser: Peter Ehrhard (Universität Dortmund, Germany)
Co-organiser: Ewald Krämer (Universität Stuttgart, Germany)
Co-organiser: Guenter Brenn (TU Graz, Austria)

Investigations on damping behaviors of lateral excited liquid in cylindrical propellant vessels. **Tim Arndt** (Universität Bremen, Germany) GA/CT2344/010

Liquid sloshing represents an undesired phenomenon concerning most applications for fluid management in Space Transportation Systems (STS). Since the liquid propellant necessary to boost the STS from Earth surface to its orbital position is the most significant weight fraction influencing the attitude control, in particular the damping behavior of excited space propellant is from major interest. In our current work, we investigate the experimental damping behaviors using cylindrical tank geometries including the most prevalent flat, convex, and concave bottom profiles. During the experiments, the test liquid is driven close to their eigenfrequencies for certain fill levels. Then, the excitation is stopped, so that the sloshing

motion can decay. Damping characteristics are determined from sloshing forces that are acquired by load cells under the tank and from wave amplitudes mapped by the sloshing liquid surface on the tank wall. As a result, it can be shown, that the damping characteristics of sloshing liquid are directly connected to the varied fill level for all applied vessel geometries. Our conclusions are correlated to numerical simulations using commercial CFD solver.

A stall delay model for rotating blades. **Horia Dumitrescu** (Romanian Academy, Bucharest), Vladimir Cardos (Romanian Academy, Bucharest) GA/CT626/010

Even for the case of quasi-steady conditions the aerodynamic forces on a radial strip of the blade can be different than equivalent two-dimensional forces derived from two-dimensional wind tunnel tests or two-dimensional calculations. This difference is often called a three-dimensional effect, than can have several causes. Firstly, a wind turbine blade has a finite length and there will be end effects at the tip and at the root. The effect of finite span results in lower aerodynamic forces and appears in both non-rotational and rotational conditions. Therefore, this could be called non-rotational three-dimensional effect, essentially of non-viscous nature. But, what is more important for a wind turbine blade is the three-dimensional effect or rotation. The blade rotation causes large span-wise pressure gradients and the flow will be affected by centrifugal and Coriolis forces. This results in the augmentation of aerodynamic forces and could be called rotational three-dimensional effect, essentially of viscous nature. The paper investigates the boundary-layer characteristics on a wind turbine blade of small chord length. The three-dimensional form of momentum integral equations is derived and used to predict the boundary-layer growth and limiting streamlines angles on the blade surface for both attached and separating flow. The chordwise skin friction coefficient is used to identify boundary layer separation and shear layer reattachment locations. The nature of flow near to the axis of rotation is discussed ad a stall-delay is proposed.

Fluctuation measurements in the boundary layer of a supersonic flow. **Birgit Lenz** (Universität Stuttgart, Germany), Uwe Gaisbauer (Universität Stuttgart, Germany), Ewald Krämer (Universität Stuttgart, Germany) GA/CT3816/010

In recent years, a special constant temperature hot-wire anemometer (CTA) has been developed at the Institute of Aerodynamics and Gas Dynamics (IAG) of Stuttgart University in cooperation with the company Cosytech GmbH and the Institute of Theoretical and Applied Mechanics (ITAM) in Akademgorodok, Russia. This anemometer features a high cut-off frequency and the possibility to switch between a certain number of preset overheat ratios in a scanning procedure. Due to the dependence of the hot wire's sensitivity towards mass flow and total temperature fluctuations on overheat ratio, these quantities can be determined in one single measuring step. Additionally, the fluctuation levels of pressure, density and velocity may be calculated by Kovásznay's modal analysis.

The application of the hot-wire anemometer inside the boundary-layer afforded certain corrections in the data analysis developed for free-stream measurements: Firstly, the existing model for the anemometer transfer function had to be extended by comprehension of inductances of cable wires, frequency-dependent gain and the hot wire time constant. Secondly, a temperature correction was introduced, to account for the non-constant total temperature profile inside the boundary layer.

Experiments took place in the middle-sized supersonic wind tunnel (HMMS) of IAG, at a Mach number of 2.5. First measurements were undertaken at a flat plate, subsequent ones are taken in the near-shock region at a ramp configuration. For necessary corrections in the CTA hot-wire analysis, the profile of the boundary layer was determined simultaneously to the fluctuation measurements at the correspondent wall distance. Hereby, the temperature profile was achieved via a cold wire and the velocity profile via a Pitot tube.

GA/CTS4878/10: Flow stability and transition.

Organiser: Ewald Krämer (Universität Stuttgart, Germany)
Co-organiser: Guenter Brenn (TU Graz, Austria)

Stability analysis of the flow in a wetting/dewetting (micro-)gap. **Peter Ehrhard** (Universität Dortmund, Germany), Sabine Strein (Forschungszentrum Karlsruhe, Germany) GA/CT3477/010

Dynamic wetting or dewetting is important in many technical coating processes, like the production of photographic films or liquid-crystal displays (LCDs). In these production processes, for economical reasons, a fast and steady coating of a liquid onto a solid is of great importance. In such coating processes, however, an unstable contact line is observed beyond a critical coating velocity, causing air entrainment and, subsequently, a poor quality of the coating layer. In detail, the straight dynamic contact line takes a saw-tooth form in this unstable regime. This instability of the contact line may be caused by the instability of the flows on either side of the interface. For a prediction of the critical velocity, hence, it appears desirable to evaluate the stability of these flows.

In this study we concentrate on the flow in the convergent gap between the moving substrate (solid) and the free interface. This flow is responsible for the removal of air from the substrate, before the liquid can contact the substrate. The base flow is considered two-dimensional, steady and incompressible, featuring two basic pattern. In a first step we idealize the free interface as geometrically-fixed and approximate the kinematic boundary conditions reasonably. The idealized base flow is subjected to small 3-D and time-dependent perturbations. The governing equations are mass and momentum conservation, formulated in cylindrical coordinates within a radially-unbounded domain. We discuss stability results, obtained for various base flows and various geometric forms of the free interface. Further, an outlook towards a more precise modeling of the free interface is given.

Towards the problem of hydrodynamic stability of dispersed flows. **Alexander Osiptsov** (Moscow State University, Russian Federation), Sergei Boronin (Lomonosov Moscow State University, Russian Federation) GA/CT639/010

In the framework of a two-fluid model, we consider the linear stability of three plane-parallel flows of a viscous fluid with spherical inclusions, namely, a two-phase boundary layer on a flat plate and upward and downward channel flows of a viscous dusty gas in the presence of the gravity force. In the classic formulation of the linear stability problem given by P. Saffman for dusty flows in 1961, only the Stokes drag was taken into account in the interphase momentum exchange and, in the basic steady-state flow, phase velocity slip and particle concentration nonunifromities were neglected. The aim of our study is to develop the formulations of the linear-stability problem for dispersed flows with account for possible nonuniformities of the basic particle concentration profile, shear-induced lifting forces acting on the particles in locally shear flows, and

a possible phase velocity slip in the basic flow. For the flows considered, linearized equations of the two-fluid model are reduced to a modified Orr-Sommerfeld equation with several extra terms describing the feedback effect of the particles on the carrier flow, which significantly complicate the traditional formulation of the problem. The corresponding eigen-value problem is solved using an orthonormlization method with controlled accuracy. A parametric study of neutral-stability curves is performed. It is shown that the new factors considered may drastically change the limits of the laminar flow regime even at fairly small particle mass concentrations. For instance, in the two-phase boundary layer the lifting forces may result in the splitting of the instability region and a sharp decrease in the critical Reynolds number, while in the downward channel flow the gravity-induced velocity slip may result in the complete suppression of small perturbations. The problem of so-called critical layers will also be discussed in the presentation.

Instability mechanisms in bouyant-thermocapillary liquid pools. **Ulrich Schoisswohl** (TU Wien, Austria), Hendrik Christoph Kuhlmann (TU Wien, Austria) GA/CT3319/010

A cylindrical volume of fluid, with a free surface on top, is heated by a parabolic heat flux from above. Two physical effects drive a bouyant-thermocapillary flow. On the one hand temperature gradients on the free surface, introduced by the heat flux, and on the other hand bouyancy forces, due to gravity. The basic axisymmetric flow is computed by finite volumes and its stability is investigated by a linear stability analysis. It is found that the critical stability boundaries and the critical modes are quite similar to those which are well-known from the half-zone model of crystal growth.

For low Prandtl numbers the critical mode is steady and three-dimensional. We find an asymptotic critical value in the limit of vanishing Prandtl number. For increasing Prandtl number the critical Reynolds number increases. Near unit Prandtl number no threshold could be found with the present computational limitations. For Prandtl numbers larger than unity, the critical mode is oscillatory and the critical Reynolds number decreases with the Prandtl number. The low- and high-Prandtl-number instabilities are caused by different instability mechanisms. We present evidence that the low-Prandtl-number instabilities are essentially centrifugal and that the high-Prandtl-number instabilities are due to the hydrothermal-wave mechanism.

Experiments on the transition to 3D-flow structures in two-sided lid-driven cavities. **Tanja Siegmann-Hegerfeld** (TU Wien, Austria), Stefan Albensoeder (Universität Bremen, Germany), Hendrik Christoph Kuhlmann (TU Wien, Austria) GA/CT2869/010

Flow instabilities in two-sided lid-driven-cavities are investigated. The flow is driven by the tangential motion of two opposite walls which are realized by cylinders of large radii in the experimental setup. The transition of the nearly two-dimensional flow to three-dimensional flow structures is investigated for the one-sided, the parallel and the anti-parallel motion of the driven walls. The Reynolds numbers of both sides have been varied between ± 1200. The geometry is characterized by the cross-sectional aspect ratio Γ and the spanwise aspect ratio Λ. Two aspect ratios ($\Gamma = 1$ and $\Gamma = 0.76$) have been investigated. The spanwise aspect ratio of $\Lambda > 10$ is sufficiently large to to minimize end-wall effects. Qualitative results have been obtained by using visualization techniques. Furthermore, LDA and PIV measurements have been conducted to obtain quantitative results. Depending on the Reynolds numbers nearly two-dimensional steady flows as well as steady and time-dependent three-dimensional flows are analyzed. We have characterized six different three-dimensional flow pattern. Each of them corresponds to a certain critical mode of previous numerical stability analyses. In most cases the experimental critical Reynolds numbers, flow structures, velocity profiles, and bifurcation diagrams are in very good agreement with the corresponding numerical predictions.

A preliminary study of the effect of the external stream structure on turbulent spots generation during bypass transition. **Pavel Jonas** (Institute of Thermomechanics Academy of Sciences, Czech Republic), Witold Elsner (TU Czestochowa, Poland), Marian Wysocki (TU Czestochowa, Poland), Vaclav Uruba (Czech Academy of Sciences, Czech Republic), Oton Mazur (Institute of Thermomechanics Academy of Sciences, Czech Republic) GA/CT1826/010

It was clearly proved that not only the turbulence level of the external flow but also the turbulence length scale influence the start and the end of boundary layer by-pass transition; e.g. Jonas et al., Eur. J. Mech. B Ű Fluids 19, 2000, 707-722. An elaborated physical notion on the role of the external turbulence length scale in transition process is not yet available. The characteristic feature of laminar-turbulent transition process is the appearance of turbulent spots followed by calmed regions, well defined structures that dominate the last stage of transition. So the investigation of the formation and development of turbulent spots can explain the effect of length scale on transition process. The experiment was executed on a flat plate boundary layer at different external flow turbulence scales of velocity and length (ERCOFTAC Test Case T3A+). Special methods were developed and applied for the instantaneous wall friction measurement and for the conditional analysis of wall friction records. Additionally, a special spot detection method developed by Elsner et al., Chemical and Process Eng. Vol. 27, 2006, 935-950 was applied. This method utilizes a wavelet analysis to detect particular frequency components and to localize spot occurrences in time.

Experiments on the laminar/turbulent transition of liquid flows in rectangular micro channels. **Peter Ehrhard** (Universität Dortmund, Germany), Wolf Wibel (FZ Karlsruhe, Germany) GA/CT3480/010

The advances of micro-fabrication techniques allow for the manufacturing of micro heat exchangers or micro reactors. These micro devices are characterized by a large surface-to-volume ratio and, hence, allow for the transfer of large heat fluxes or offer large katalytic surfaces for reactions. The design and optimization of such micro devices heavily relies on correlations for pressure drop and heat transfer, as well as on information on the laminar/turbulent transition. As these questions are still discussed controversially in literature, a careful investigation appears highly desirable.

We concentrate onto rectangular stainless steel micro channels with a hydraulic diameter of $d_h \simeq 133\,\mu\mathrm{m}$. Three aspect ratios are engaged, namely 1:1, 1:2, 1:5, whereas the hydraulic diameter is kept constant. The roughness of the channel walls is $k \simeq 1\text{–}2\,\mu\mathrm{m}$ in general, specific channels are of roughness $k \simeq 25\,\mu\mathrm{m}$. Filtered and degassed de-ionized water is driven at pressure differences up to $20\,\mathrm{bar}$ through the channels, allowing for Reynolds numbers up to $\mathrm{Re} \simeq 4000$. The measuring techniques allow for a highly-accurate determination 1. of the mass flow rate (precision weighting), 2. of the temperatures at inlet and outlet, 3. of the pressure drop, and 4. of the time-resolved velocity field (μPIV).

We find from all measured quantities, consistently, the laminar/turbulent transition for smooth channels in the range $\mathrm{Re}_c \simeq 1900\text{–}2200$, in agreement with findings for macroscopic channels. The influence of rough channel walls appears particularly strong for the micro channels of aspect ratio 1:5 ($\mathrm{Re}_c \simeq 900$). This raises the question, whether the dimensionless group (k/d_h) remains the relevant parameter at extreme aspect ratios.

GA/CTS4877/10: Thin films and biomedical flows.

Organiser: Ulrich Rist (Universität Stuttgart, Germany)
Co-organiser: Ewald Krämer (Universität Stuttgart, Germany)
Co-organiser: Guenter Brenn (TU Graz, Austria)

Capillary hydrodynamics of the deposition of thin liquid films and droplets on heterogeneous, porous substrates. **Daniel Gerlach** (Universität Erlangen–Nürnberg, Germany), Norbert Alleborn (Universität Erlangen–Nürnberg, Germany), Antonio Delgado (Universität Erlangen–Nürnberg, Germany), Hans Raszillier (Universität Erlangen–Nürnberg, Germany) GA/CT4112/010

The paper to be presented will deal with recent research work on capillary hydrodynamics of thin viscous liquid films and droplets. The process engineering background comes from industrial processes to deposit thin films or droplets on substrates such as polymer foils or paper [1].

In the first part, the fluid dynamics of thin viscous liquid sheets, which are used to deposit liquid films in curtain coating, is investigated. The focus will lie on the propagation of disturbance signals in a uniformly thin viscous liquid sheet of infinite extent which is in contact with a passive ambient medium. The disturbances considered are induced by local external pressure perturbations moving on the sheet interfaces. The tool of analysis is the Fourier-Laplace transform of the linearized perturbation equations, and the inverse Fourier-Laplace transform for the numerical reconstruction of the amplitude of the interface deflections. Symmetric (varicose) and antisymmetric (sinuous) disturbances are investigated in the long time limit by numerical signal evaluation. The exact disturbance responses are compared with their longwave approximations [2].

The second part will investigate the fate of films and droplets on heterogeneous, porous substrates *after* their deposition in a coating process. Besides the fluid dynamics *on top of* the substrate, the capillary transport of fluid *inside* the porous substrate will be considered. The dynamics of the fluid on the substrate surface is treated in the framework of lubrication approximation. Fluid flow within the porous substrate, caused by the droplet penetrating into it, is treated in the framework of Richards' equation, which models *unsaturated flow* in porous media. Numerical results for sorption of films and droplets into a substrate of finite thickness show the influence of the sorption characteristics of the porous material on the final fluid distribution within the substrate. The interplay of fluid properties and wetting and sorption properties of the substrate hereby offers the possibity of a controlled structuring of surfaces, e.g. in microsystem technology [3].

[1] N. Alleborn. Progress in Coating Theory. *Thermal Science*, 5:131–152, 2001.

[2] N. Alleborn and H. Raszillier. Linear response of a viscous liquid sheet to oscillatory external pressure perturbation in the long wave approximation. Varicose excitation. *Acta Mechanica*, 170:77–119, 2004.

[3] N. Alleborn, H. Raszillier. Spreading and sorption of droplets on layered porous substrates. *J. Colloid Interface Sci.*, 280:449–464, 2004.

Influence of the bottom undulation on surface waves in thin film flows. **Christian Heining** (Universität Bayreuth, Germany), Andreas Wierschem (TU München, Germany), Nuri Aksel (Universität Bayreuth, Germany) GA/CT2149/010

We study viscous gravity-driven thin films flowing down an undulated plane. Applying the integral boundary-layer method we derive a set of coupled PDEs for the film thickness and the flow rate. The steady state solution shows linear and nonlinear resonance. Based on this analytical solution we carry out a stability analysis with respect to surface waves and study wave generation and annihilation.

Soap bubbles: an illustration of potential flow theory and the Dirichlet problem. **Josué Sznitman** (ETH Zürich, Switzerland), Thomas Roesgen (ETH Zürich, Switzerland) GA/CT2381/010

There are few physical objects as beautiful and fascinating as soap bubbles. They exhibit a perfection of geometrical form and an appealing simplicity. Soap bubbles are characterized by the structure of their thin liquid shell of low surface tension. It is well known that the dynamics of the surface of soap bubbles are the resultant of both 1) liquid film thinning under the influence of gravity, and 2) the presence of local surface tension gradients which create complex flows (Marangoni flows). In turn, the net motion of the thin liquid shell induces the displacement of gas inside the cavity due to the no-slip boundary condition which holds at the liquid-gas interface. Both flows on the liquid shell and within the cavity are incompressible. Moreover, the boundary-driven internal cavity flows are viscosity-dominated such that they are effectively governed by the equations of creeping motion.

While soap bubbles exhibit intrinsic internal flows, thermally-induced Marangoni flows in the liquid film may lead to steady-state forced recirculation inside the cavity. Experimentally, this may be achieved by applying a thermal gradient in the vicinity of the liquid shell. Because most liquids maintain a negative and constant value of $d\sigma/dT$, where σ is the surface tension and T the temperature, the application of a constant thermal gradient produces a fixed shear stress at the liquid surface given by $\tau = \mathrm{d}\sigma/\mathrm{d}\underline{x} = (\mathrm{d}\sigma/\mathrm{d}T)(\mathrm{d}T/\mathrm{d}\underline{x})$, where $\underline{x}$ relates to the spatial direction. Thus, a fixed-shear stress on the shell boundary will lead in turn to steady-state flows in the liquid shell and within the cavity itself following conservation of mass. In the present discussion, we will show experimental flow visualizations of the boundary-driven cavity flows inside soap bubbles, which may be controlled by such thermal forcing schemes. Variations in the number and location of heat sources applied near the liquid shell effectively yield different internal flow topologies. Such steady-state flows on the surface of the shell and within the soap cavity may be mathematically modeled using potential flow theory by solving the Laplace equation, $\triangle\Phi = 0$, for the flow potential Φ on the boundary and within the cavity. In particular, soap bubbles illustrate here the well-known Dirichlet problem for a sphere, where flow on the boundary of the sphere is prescribed by the forced motion of the liquid shell and flow within the spherical boundary is then solved for.

Finite-volume simulation of blood flow through complete bypass models. **Jan Vimmr** (University of West Bohemia, Czech Republic), Alena Jonášová (University of West Bohemia, Czech Republic) GA/CT2498/010

It is proven that the *intimal hyperplasia* (IH) is the main reason for the late failure of bypass grafts due to the restenosis of the anastomosis between the graft and the blood vessel. Hence the influence of hemodynamics on the occurrence of IH should be analyzed in form of recirculation zones, eddies, low and oscillating Wall Shear Stress (WSS) and large spatial Wall Shear Stress Gradient (WSSG). In this study these factors are analyzed for a blood flow through a 2-way bypass graft in comparison to the traditional 1-way bypass graft. The effect of the junction angle and bypass graft diameter in both types is observed by various degree of stenosis of the host tube including the fully blocked case as the final phase of the atherosclerosis.

The problem of the blood flow through a complete bypass model with rigid walls is solved as an isothermal laminar flow of viscous Newtonian fluid using the incompressible Navier-Stokes equations. The calculations are based on the cell-centered finite volume method. The time marching scheme employs a predictor-corrector technique using a variable time step. The traditional 1-way bypass model is based on the study elaborated by Lee et al. (2001), which includes the proximal and distal parts of the host tube together with the end-to-side bypass graft. The resulting velocity and pressure distributions in the idealized models are obtained for steady and physiological pulsatile flows by varying Reynolds and Womersley numbers.

Numerical simulation of the endolymph flow in the semicircular canals of the vestibular organ. **Dominik Obrist** (ETH Zürich, Switzerland), Leonhard Kleiser (ETH Zürich, Switzerland), Stefan Hegemann (Universitätspital Zürich, Switzerland) GA/CT1994/010

The semicircular canals are the primary human sensors for angular motion. They are part of the vestibular organ which is located in the inner ear. The semicircular canals are filled with a fluid called the endolymph. Movements of the head induce a flow of the endolymph. This flow deflects an elastic gelatinous structure (cupula). The deflection of the cupula triggers nerve signals resulting in the perception of angular motion.

A detailed understanding of the fluid dynamics of the endolymph is indispensable for the study of diseases of the semicircular canals (e.g., various forms of vertigo). Several authors have presented idealized models for the endolymph flow. All of these models, however, reduce the problem to zero- or one-dimensional equations which do not appreciate the full complexity of this configuration.

We present early results from a numerical simulation of the endolymph flow in a two-dimensional representation of the semicircular canals. Here, the endolymph flow is described as a Stokes flow in a complex annular structure, i.e., a semicircular canal. The reactive force of the elastic cupula onto the endolymph enters the Stokes equations as an external force. The highly transient character of this flow (due to the angular motion of the head and the fluid-structure interaction between the endolymph and the cupula) requires a careful treatment of the different time-scales.

The dynamics of the cupula is simulated by an explicit time-integration scheme. Within each time-step we solve the quasi-steady Stokes equations for the endolymph with the method of fundamental solutions. The transient motion of the head leads to time-dependent boundary conditions. This numerical scheme is examined for its accuracy, robustness and computational efficiency.

GA/CTS4876/10: Numerical methods.

Organiser: Olaf Wünsch (Universität Kassel, Germany)
Co-organiser: Ewald Krämer (Universität Stuttgart, Germany)
Co-organiser: Guenter Brenn (TU Graz, Austria)

Numerical solution of the incompressible Stokes equations with explicit integration of the pressure term. **Giuseppe Bonfigli** (ETH Zürich, Switzerland) GA/CT2323/010

The numerical integration of the Navier–Stokes equations for incompressible flows has always been a central topic of numerical fluid mechanics. One possible approach consists of computing the pressure p and the velocity vector $\underline{u}$ (primitive variables) at discrete grid points by solving a system of algebraic equations obtained by discretization of the governing differential equations. After discretization in time, easy analytical manipulations provide a decoupled Poisson equation for p and Helmholtz or algebraical equations, depending on the time integration scheme, for the velocity components. However, while the boundary conditions for $\underline{u}$ are clear, those for p are still subject of controversial debate.

We developed a formulation of the incompressible Navier-Stokes equations which considers boundary conditions for the p-Poisson equation obtained from the boundary-normal component of the momentum equation. The new formulation is suitable both for explicit and implicit time integration of the viscous terms, while pressure and non-linear terms are always integrated explicitly. In all cases the computational problems for the pressure and for the velocity components are decoupled. Strong similarities exist with respect to the formulation proposed by Johnston & Liu (JCP, 2004). However, our method is improved by the introduction of an additional term in the p-Poisson equation and by a new Neumann boundary condition for the boundary-normal component of the velocity. Both aspects are important to ensure the decay of eventual errors in the continuity equation.

The new formulation has been applied to the computation of a 2-D Stokes flow with unsteady boundary conditions. Spatial discretization was achieved by means of finite-differences. An explicit Runge–Kutta scheme or a semi-implicit Crank–Nicolson/Adams–Bashforth scheme were used for time integration. Convergence rates of the solution corresponded to the order of the considered discretization schemes.

High-order accurate solution of the incompressible Navier–Stokes equations. **Rolf Henniger** (ETH Zürich, Switzerland), Leonhard Kleiser (ETH Zürich, Switzerland), Dominik Obrist (ETH Zürich, Switzerland) GA/CT2382/010

We present a high-order simulation code for the incompressible Navier-Stokes equations which is suitable for massively parallel computers. It is based on a finite-difference discretization in space and a semi-implicit integration scheme in time. Velocity components and pressure are calculated on a staggered grid. The elliptical problem is solved in an iterative manner, split into inner and outer iteration cycles, such that the momentum and continuity equations are exactly satisfied. The inner iteration cycle is similar to a discrete Poisson problem with Neumann boundary conditions. We employ a multigrid procedure with either Jacobi or Gauss-Seidel smoothing for its solution. Non-periodic boundaries are handled explicitly or (partially) implicitly. In addition, the rate of convergence is accelerated by a Krylov subspace method (BiCGStab) which utilizes the multigrid algorithm as a preconditioner. We investigate the efficiency of the nested iteration cycles with respect to the timestep size, the Reynolds number, the spatial resolution and different multigrid parameters for a channel flow configuration.

Viscosity in discontinuous Galerkin methods. **Manuel Keßler** (Universität Stuttgart, Germany) GA/CT3805/010

In technical fluid applications viscosity plays an important, and often dominant, role for the flow phenomena at interest. Moreover, as these applications feature high Reynolds numbers and thus in general turbulent flow, turbulence modeling of some kind or another is the only affordable alterntive, as LES or even DNS are usually prohibitively expensive. Any approach to simulate such flows therefore needs to take viscous effects into account.

Discontinuous Galerkin (DG) methods have gained some interest in recent years, as they deliver high order on unstructured grids, have little requirements on grid quality, excellent adaptation and parallelisation properties and a computational pattern suitable for the ever spreading clusters of scalar commodity processors.

However, second and higher derivatives, and thus viscosity and turbulence models, and DG do not mix—at least not very well. The mathematical framework is rigorous for first derivatives, but basically undefined for higher ones. Fortunately, nature teaches us that the problem at hand is well posed indeed, and therefore solutions should be possible.

One remedy is to reformulate the equations as a first order system, introducing the needed derivatives as independent variables of their own. While this so-called Local DG (LDG) is the mathematically cleanest way, the explosion of solution variables—e.g. from 7 to 24 in three dimensional $k-\omega$ simulations—often is too expensive, especially for implicit time integrations, where the memory increase is even more pronounced.

Another approach starts from the same considerations, but evaluates the additional terms with some approximations for the surrounding region. The main point here, introduced by Bassi and Rebay, is to decompose the discrete derivative into a part based on the local polynomial exact derivative in the cell interior, which is easily computable, and another one caused by the discontinuity jumps between cells. The latter increases the computational stencil by the surrounding cells, but allows one to get rid of the explicit storage of derivatives and instead compute them on the fly, along with the flux computation.

Once second derivatives are integrated into the DG framework efficiently, viscous simulations are no further difficulty for DG. However, due to the high order nature of the method, modifications on the turbulence model may be beneficial, in order to take advantage of the rich structure available in the polynomial solution representation in each cell. Concept and efficiency of such modifications are an area of active research.

Numerical modelling of turbulent flow over rough walls. **Petr Louda** (CVUT v Praze, Czech Republic), Karel Kozel (CVUT v Praze, Czech Republic), Jaromír Příhoda (Czech Academy of Sciences, Czech Republic) GA/CT1679/010

The numerical simulation of turbulent flow over rough walls was carried out for various types of roughness. The mathematical model was based on the Reynolds averaged Navier-Stokes equations for incompressible flow. The two-equation k-ω/k-ϵ SST model proposed by Menter and the one-equation model according to Spalart and Allmaras were used. The system of governing equations was solved by the artificial compressibility method. The cell-centered finite volume method with the third order upwind interpolation for convection term and the second order central scheme on dual grid for diffusion terms were used for the space discretization. The time discretization was carried out by the implicit backward Euler scheme with the Newton linearized system solved iteratively. Boundary conditions on rough walls were prescribed by wall functions and/or directly on the wall using the SST model modified to account for wall roughness by Hellsten and Laine (1997) and the SA model modified by Aupoix and Spalart (2003). Turbulence models were tested for the constant-pressure turbulent boundary layer on the rough wall formed by commercial abrasive paper and by tightly-packed spheres. The dependence of the velocity shift in the logarithmical region on the wall-roughness type was studied for transitional and fully-rough regimes. Besides, the effect of wall roughness on the decelerated flow over a smoothly contoured ramp with flow separation was investigated. Obtained results were compared with experimental data.

On a new numerical algorithm for the solution of triple deck problems. **Rene Szeywerth** (TU Wien, Austria), Alfred Kluwick (TU Wien, Austria) GA/CT1845/010

A new algorithm for the solution of laminar viscous-inviscid interactions allowing for the formation of pronounced separation zones is presented. It is then applied to two different types of flows: near critical two layer fluid flow and subsonic flow past an expansion ramp. In the first case emphasis is placed on the formation of so-called non-classical hydraulic jump having the distinguishing property that waves pass through rather than merge with the jump. The second problem exhibits the interesting feature that no solution exists if the ramp angle exceeds a critical value while two solutions exists if the ramp angle is subcritical. The new numerical scheme is used to study the change in the flow behaviour as the critical ramp angle is approached.

Moving-mesh approach for solving Reynolds' bearing equation. **Bernhard Schweizer** (Universität Kassel, Germany) GA/CT4298/010

Basis of the hydrodynamic bearing theory is the Reynolds bearing equation. In its original form, the Reynolds equation is a linear partial differential equation for the calculation of the pressure distribution in the bearing. To solve this equation, boundary conditions have to be applied which must take into account cavitation effects. When using the so-called Reynolds boundary conditions, the governing boundary value problem is nonlinear. Various methods exist to solve this problem. Here, a new method based on an ALE-approach is presented.

11, Short Communications

GA/CTS4821/11: **Compressible flows, I.**

Organiser: Josef Ballmann (RWTH Aachen, Germany)

Release dynamics of liquefied gases from pressure storage tanks. **Jean Paul Kunsch** (ETH Zürich, Switzerland) GA/CT1758/011

Storage tanks with pressurized liquid gases such as propane or chlorine represent a substantial hazardous potential. The dynamics of a release through an opening or an accidentally generated puncture are studied. An important quantity to be determined is the time to empty the reservoir, since it represents the initial condition of the subsequent dispersion process. Another relevant quantity is the cooling of the liquid phase which influences the vapour pressure, which on its part represents a driving force of the outflow dynamics.

A perturbation method, taking the temperature dependence of the thermal quantities and of the vapour pressure into account, is proposed to describe the emptying of the storage tank. A first approximation based on constant vapour pressure but also higher-order solutions are presented. Their validity is discussed for commonly used gases with regard to risk assessment studies, where the release scenario represents an initial element in the chain of events.

Transonic viscous inviscid interactions in narrow channels. **Georg Meyer** (TU Wien, Austria), Alfred Kluwick (TU Wien, Austria) GA/CT1734/011

Transonic flows through channels which are so narrow that the classical boundary layer approach fails are considered. As a consequence the properties of the inviscid core and the viscosity dominated boundary layer regions can no longer be determined in subsequently steps but have to be calculated simultaneously. The resulting interaction problem for laminar flows is formulated for both perfect and dense gases. Representative solutions including the internal structure of pseudoshocks and the choking phenomenon will be presented.

Aerodynamic optimization of Laval nozzle flow with shocks: numerical investigation of active/passive shock control via expansion fans. **Nisar Al-Hasan** (TU München, Germany), Günter Schnerr (TU München, Germany) GA/CT1663/011

Instantaneous ignition in the supersonic part of a 3D Laval nozzle is realized by a well-defined sudden temperature rise across a normal shock. Unfortunately, the divergence of the supersonic nozzle part is necessarily smooth. Therefore, the turbulent boundary layer ahead of the shock is thick and causes substantial shock/boundary layer interactions. The non-homogeneous temperature increase across the shock, caused by the boundary layer thickening ahead of the shock and the resulting pre-compression prevents the quasi 1D evolution of the flow downstream. Additionally, due to the boundary layer thickness the single shock disintegrates in a so called *pseudo-shock system*; i.e., into a sequence of periodic weak compression and expansion regions.

To avoid this drawback and to establish homogeneous thermodynamic conditions throughout the entire cross section and flow domain downstream of the shock we apply active and passive control techniques in the area of shock boundary/layer interaction. The central idea of the control technique described below is compensation of the thickening of the boundary layer by quantitative appropriate inverse effects, i.e. by superimposing negative and positive pressure gradients in the near wall region close to the shock position.

In a first approach the additional expansion fan is created by active suction slots in flow direction and through all sidewalls of the 3-D nozzle. The resulting shock remains straight with exception of the near wall region. Suction creates an effective convex wall curvature. In supersonic flow the resulting local expansion tends to compensate the pre-compression. Because suction in high temperature environment is difficult to realize, we alter the wall curvature to create a *negative bump* with the same effect on the effective wall curvature. Under these conditions a single plane normal shock could be established without active or passive suction. The paper presents parameter studies for optimization of the operating conditions.

The effect of shock-wave/boundary-layer interaction on turbulent spot propagation. **Andreas Jocksch** (ETH Zürich, Switzerland), Leonhard Kleiser (ETH Zürich, Switzerland) GA/CT2499/011

We performed highly resolved Large-Eddy Simulations of transitional shock-wave/boundary-layer interactions (SW/BLI) in which a turbulent spot passes through a laminar shock-induced separation bubble. For discretisation we employ a sixth-order compact finite-difference scheme in space and a third-order Runge-Kutta time-marching scheme. Unresolved scales are treated by the Approximate Deconvolution Model using the relaxation term only (ADM-RT). The LES model is also engaged to handle the shock. The initial condition consists of a laminar boundary-layer solution on a flat plate with a superimposed oblique shock which induces a separation bubble on the plate. An upstream-positioned initial disturbance consisting of a localised vortex pair triggers the turbulent spot that develops downstream and eventually encounters the SW/BLI region. The separation bubble collapses during the spot passage and regains its undisturbed shape after the spot has passed. Unlike the laminar boundary layer, the turbulent region does not separate in the shock region. This phenomenon is described as tunneling of the turbulent spot through the SW/BLI region. Compared to a simulation without SW/BLI, the spot growth is increased significantly during the shock-region passage. Despite this influence, the characteristic shape of the spot is qualitatively maintained. This finding supports the results of previous DNS by Krishnan and Sandham (2004).

Large-eddy simulation of film-cooling. **Jörg Ziefle** (ETH Zürich, Switzerland), Leonhard Kleiser (ETH Zürich, Switzerland) GA/CT2476/011

In modern high-performance gas turbines, the hot gas from the combustor enters the turbine stages at temperatures that often exceed the material limits of the turbine blades. Therefore, they have to be protected, which is usually done by a technique called film-cooling in which a layer of cool air ejected through small holes near the leading edge of the blades shields their surface.

We performed time-dependent three-dimensional numerical simulations of the well-known film-cooling configuration of Sinha *et al.* In their experiments cold fluid was ejected through a row of short oblique nozzles into a relatively hotter turbulent adiabatic flat-plate boundary-layer. Our flow parameters were chosen according to case 10 of Sinha et al., with a jet-to-crossflow density ratio of 2, a jet-to-crossflow velocity ratio of 0.25, and a Reynolds number of 15875 (computed with the jet diameter and free-stream quantities). The non-resolved turbulent flow scales are taken care of by the approximate deconvolution model (ADM). In previous work, this subgrid-scale model was implemented into the simulation code NSMB, a finite-volume solver for the compressible Navier-Stokes equations. NSMB supports domain decomposition using grid blocks and is MPI-parallelised on the block level. In a series of LES of separated flow configurations with increasing complexity, the ADM code has been successfully validated and proven to work

very well for compressible flows featuring strong unsteady vortical structures.

The goal of this study is to evaluate the performance of the approximate deconvolution model for film-cooling applications, and to investigate the suitability of the simulation approach and the employed simplifications, e.g. the use of a mean turbulent boundary-layer profile instead of unsteady turbulent inflow data. Special focus is placed on the mixing properties in the near-field of the orifice as well as on the influence of buoyancy. We will support our findings with detailed visualisations of the three-dimensional time-dependent flow field, especially the vortical structures in the mixing region. Furthermore, we will study the flow conditions in the jet nozzle, especially the secondary flows, which are known to have a strong influence on the downstream mixing behaviour and thus the cooling efficiency.

Assessment of high-order discretization schemes for computation of compressible swirling mixing layers. **Sebastian Müller** (ETH Zürich, Switzerland), Leonhard Kleiser (ETH Zürich, Switzerland) GA/CT2401/011

We report on results obtained with a highly accurate Direct Numerical Simulation (DNS) and Large-Eddy Simulation (LES) code solving the (filtered) Navier-Stokes equations in cylindrical coordinates. The code computes a compressible swirling mixing layer (i.e. a circular mixing layer with an additional swirl component which is present only in the shear layer) at Mach number $Ma = 0.8$. This flow incorporates the nonlinear disturbance development and transition to turbulence of the laminar layer perturbed at the inflow by viscous spatial instabilities.

We will present two simulations differing in the spatial discretization schemes for the convective terms. One discretization is based on up to tenth order central compact finite differences in the radial and axial directions and a Fourier spectral method in the azimuthal direction, combined with an additional secondary filter operation (corresponding to $\hat{Q}_5\hat{G}$ in the ADM relaxation term) every second time step to ensure numerical stability. The other discretization uses upwind-biased schemes in all spatial directions.

Apart from varying the grid resolution, comparisons of flow simulations using different discretization schemes for otherwise identical conditions can be performed quantitatively and improve the understanding of the effects of numerical errors and in particular numerical dissipation. Furthermore they may contribute to improved estimates concerning resolution requirements in general flow situations.

The differences of the computational schemes will be shortly outlined. We will focus on detailed comparisons concerning flow statistics as well as on highlighting the small scale structures.

GA/CTS4822/11: Compressible flows, II.

Organiser: Leonhard Kleiser (ETH Zürich, Switzerland)
Co-organiser: Josef Ballmann (RWTH Aachen, Germany)

On fluid-structure interaction in transonic wind tunnels. **Bosko Rasuo** (University of Belgrade, Yugoslavia), Aleksandar Bengin (University of Belgrade, Yugoslavia) GA/CT894/011

This paper studies the interaction (influence) of perforated walls of transonic wind tunnels in two-dimensional investigations which employ the generalized method for solving DirichletŠs problem formulated for the rectangle of the transonic wind tunnel work section. In order to preserve the realistic features of the flow at the work sectionŠs perforated boundaries, the boundary conditions, which are required to solve this type of boundary problem, are experimentally determined by measuring the static pressure distribution in the vicinity of the walls of the work section. The algorithm has been applied to the aerodynamic experimental results from investigations of NACA 0012 airfoil obtained at the VTI -Aeronautical Institute and the Faculty of Mechanical Engineering in Belgrade to demonstrate in two-dimensional investigations the appropriateness of the presented advanced algorithm for the calculation of the interference of the transonic wind tunnel wall.

Aerodynamic characteristics of the propeller in non-axial flow. **Milan Vrdoljak** (University of Zagreb, Croatia) GA/CT3794/011

Flow on running propellers installed on aircraft in general case is not axial. This results in off-axis forces and moments at propeller which are treated here in form of aerodynamic coefficients. Importance of forces and moments of propeller in non-axial flow lies in the fact that they have significant influence on aircraft static stability.

Presented numerical model of the propeller is based on the vortex theory and it includes model of propeller wake. Lifting line method is applied for propeller blade model using set of discrete Π vortices. Free-wake method with relaxation technique is applied for determination of propeller wake described with discrete vortices forming vortex sheet from each propeller blade. Using this approach for propeller vortex wake roll-up, segments of blade trailing vortices coincide with streamlines. Since the results for blade circulation distribution are directly connected to the geometry of its vortex wake, complete model of propeller is composed of blade model and wake model which are applied successively.

Given model is applied for analysis of aerodynamic characteristics of a propeller under the angle of attack, or sideslip angle, or their combination. Results of presented model for off-axis forces and moments coefficients of propeller in non-axial flow are compared with experimental results and other analytical methods for particular propeller geometry. Presented low computational cost numerical model is suitable for implementation in component build-up method and could be used for prediction of propeller contribution to the aircraft aerodynamic characteristics.

New developments regarding supersonic flows over delta wings with supersonic leading edges. **Stefan Mihai Neamtu** (INCAS, Bucharest, Romania) GA/CT3196/011

Compact expressions of the perturbation velocities over delta wings with supersonic leading edges and their application for wing aerodynamic characteristics calculation are presented. The new expressions are developed in the framework of small perturbation conical flow theory and cover conical delta wing configurations of high order. The present abstract will be completed later with further details.

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GA/CTS4837/12: **Waves and acoustics, II.**

Organiser: Reinhard Lerch (Universität Erlangen–Nürnberg, Germany)
Co-organiser: Wolfgang Schroeder (RWTH Aachen, Germany)

Numerical eigen-mode analysis of an acoustic-duct system by CFD-OLG and comparison against experiment. **Urban Neunert** (TU München, Germany), Jan Kopitz (Universität München, Germany), Thomas Sattelmayer (TU München, Germany), Wolfgang Wolfgang Polifke (TU München, Germany) GA/CT2153/012

Duct systems in engineering applications can be prone to wanted or unwanted acoustic resonances. Numerical methods are required to predict these phenomena in early design stages. One such method to describe the acoustic properties of an acoustic system is the 1-D network model, which combines the acoustic transfer matrices of all elements representing the system. Since the transfer matrices of all system elements have to be known, this method is often limited.

Another possibility is to simulate the complete system with compressible CFD. Although this allows the prediction of the acoustic behaviour of even highly complex geometries very precisely, it inevitably leads to often forbiddingly heavy computing efforts and high costs.

In previous work a combination of both methods has been presented, which combines their advantages and avoids the respective disadvantages. One rather small part of the system containing a complex element is simulated by detailed CFD with a non-reflecting boundary condition. The system answer is post-processed by a network model representing the other, geometrically rather simple, part of the system. The acoustic stability analysis is finally performed by determining the open-loop-gain.

The present work demonstrates the full capabilities of the CFD-OLG method by applying it to a complex geometry consisting of two ducts and a sudden change of area. The results are compared with analytical results and validated against experimental data. Very good agreement is achieved between the experimental results and those of the CFD-OLG method while the traditional network model is not able to match the quality of this agreement.

A multiple scales solution to the undular hydraulic jump problem. **Richard Jurisits** (TU Wien, Austria), Wilhelm Schneider (TU Wien, Austria), Yee Seok Bae (Changwon National University, Sud-Korea) GA/CT2253/012

Recently a steady-state version of a perturbed Korteweg–de Vries equation was proposed to describe the fluid's surface elevation in phenomena like the undular hydraulic jump in turbulent open channel flow. We consider the an equation of the form:

$$H''' + (H-1)H' - \beta H + \gamma = 0\,,$$

where H is the surface elevation as a function of the non-dimensional longitudinal downstream coordinate, β describes frictional damping and γ is a gravitational forcing term.

Exploring numerically the solutions of this in the parameter space (γ/β, $H(0)$, $H'(0)$ and $H''(0)$) one finds undular shapes of the surface with slowly changing amplitudes and wavelengths as well as singular surface shapes. To gain insight into the structure of the solutions, an asymptotic analysis for small values of β and γ is presented. A multiple scales approach is pursued, and the resulting undular solutions for the surface elevation are found to agree very well with numerical solutions. It is also shown that the singularities of the numerical solutions are associated with a breakdown of the corresponding undular asymptotic solutions. Considering the analytical properties of the multiple scales solution, sufficient conditions for the formation of an undular jump are obtained. Furthermore, the asymptotic behaviour of the undular jump solutions far downstream is investigated.

Finally, for the purpose of comparison, the full equations of motion of turbulent free-surface flow were solved with a commercial CFD-code using the standard $k-\varepsilon$ model. Based on an asymptotic analysis, an iteration scheme for the free surface was developed and successfully applied. The results of the analysis are also compared with experimental data, and satisfactory agreement is achieved.

Application of the Green's function technique and the modal analysis to predicting noise from a compact region of turbulence in a circular pipe. **Andriy Borisyuk** (Institute of Hydromechanics, Kiev, Ukraine) GA/CT413/012

A problem of noise production by a compact region of turbulence in an infinite straight rigid-walled pipe of circular cross-section is considered. The problem is solved via the use of the Green's function technique and the modal analysis. A turbulence region is modelled by the distributed quadrupole and dipole sources (whose characteristics are assumed to be known), and the cases of homogeneous and non-homogeneous turbulence are considered.

It is shown that the noise power does not decrease as the distance from the turbulent sources increases, and is a sum of the powers of the pipe acoustic modes. The acoustic mode power consists of the three parts. The first part is the power generated by the volume quadrupoles, the second part results from the surface dipoles, and the third part is due to interaction of the quadrupoles and dipoles. An order of magnitude analysis of these parts is carried out for different values of the flow Mach number, and the corresponding simplified expressions for the acoustic power are obtained.

Plate wave-scattering phenomena observed with pulse ESPI. **Alexander Schmidt** (Universität der Bundeswehr Hamburg, Germany), Rolf Lammering (Universität der Bundeswehr Hamburg, Germany) GA/CT1958/012

The experiments presented are part of investigations which focus on the assessment of capabilities of the *Electronic Speckle Interferometry* (ESPI) for general damage and flaw detection in structural health monitoring (SHM) and nondestructive testing (NDT).

The employed double-pulse ESPI system allows for non-contact measurements of spatially large fields of out-of-plane displacements with a resolution at least in the order of the laser wavelength. It is especially suited for measurements of transient processes or vibrations and is therefore highly unsusceptible to environmental interferences.

As test specimens, several $1000 \times 1000 \times 5mm$ steel plates are chosen with artificial flaws of different sizes, depths, and orientations. These flaws are not visible at the surface observed. The plate waves are excited by time harmonic bursts from piezo-transducers or by impact.

Experimental results will be shown, namely phase diagrams and displacement fields which are obtained from postprocessing procedures. These results include information about the location and the size of the flaws and allow for an assessment of the ESPI technique with respect to SHM and NDT. The propagation of surface waves in thin plates and the scattering phenomena with several configurations of artificial flaws are considered as first steps toward the intended later use of specific Lamb-wave modes with ESPI for SHM and NDT.

GA/CTS4836/12: Waves and acoustics, I.

Organiser: Wolfgang Schroeder (RWTH Aachen, Germany)
Co-organiser: Reinhard Lerch (Universität Erlangen–Nürnberg, Germany)

Acoustic scattering by a thin cylindrical screen with Dirichlet and impedance boundary conditions on opposite sides of the screen.
Pavel Krutitskii (Keldysh Institute of Applied Mathematics RAS, Russian Federation), Valentina Kolybasova (Lomonosov Moscow State University, Russian Federation) GA/CT2632/012

A problem on scattering acoustic waves by a thin cylindrical screen is studied. In doing so, the Dirichlet condition is specified on one side of the screen, while the impedance boundary condition is specified on the other side of the screen. The solution of the problem is subject to the radiating condition at infinity and to the propagative Helmholtz equation

$$\Delta u + k^2 u = 0, \quad k = \operatorname{Re} k > 0.$$

By using the potential theory the scattering problem is reduced to a system of singular integral equations with additional conditions. By regularization and subsequent transformations, this system is reduced to a vector Fredholm equation of the second kind and index zero. It is proved that the obtained vector Fredholm equation is uniquely solvable. Therefore the integral representation for a solution of the original scattering problem is obtained. The computational methods for finding the numerical solution are discussed.

Acoustic simulations with higher order finite and infinite elements.
Otto von Estorff (TU Hamburg–Harburg, Germany), Jan Biermann (TU Hamburg–Harburg, Germany), Steffen Petersen (TU Hamburg–Harburg, Germany) GA/CT2893/012

In recent years, the need of numerically solving the Helmholtz equation in the mid and high frequency range constantly increased. However, the efficiency of the numerical treatment of those problems is derogated by two facts: First, the numerical solution suffers from the so-called pollution effect, which gives rise to either very high element resolutions or to p-FEM concepts. Second, the resulting systems of equations are usually very large and call for the usage of iterative solution procedures, such as Krylov subspace methods. With increasing wave numbers, however, the deterioration of the spectral properties of the resulting system matrices affects the convergence and stability of those iterative solvers.
Generally, it is known that if higher order elements are used, the choice of the polynomial approximation function space is influencing the eigenvalue distribution of the resulting matrices and therewith the solution efficiency. In the present contribution the influence of different types of polynomial basis functions on the efficiency and stability of interior as well as of exterior acoustic simulations is analyzed. The investigations will show that a proper choice for the polynomial shape approximation may significantly increase the performance of Krylov subspace methods. In particular, the efficiency of higher order finite and infinite elements based on a Bernstein polynomial shape approximation and the corresponding iterative solution strategies are assessed. Moreover, practically relevant numerical examples including the sound radiation from rolling tires will show the efficiency of these 'Bernstein elements'.

Analytical modelling of active vibro-acoustic control.
Stefan Ringwelski (Universität Magdeburg, Germany) GA/CT3975/012

In recent years acoustic noise reduction has become an important concern in many industrial applications. Noise reduction increases the comfort of a system and reduces the noise radiation into the environment. The usual way to reduce the vibration and noise level of a structure is the application of additional damping materials. An alternative way for decreasing the vibration and noise emission results through the use of smart structures. A smart structure consists of a passive mechanical structure and integrated active materials, which in connection with an associated controller minimize unwanted vibration and sound radiation.

Usually the design process of a smart structure is based on numerical methods. In order to verify numerical techniques, experimental and analytical reference solutions are required. For this purposes the present paper derives an analytical reference solution for an active vibroacoustic system. The analytical model consists of a cavity coupled with a rectangular plate, which contains piezoelectric patch actuators and sensors. Based on the classical Kirchhoff equation, the transverse motion of the vibrating rectangular plate is described. The sound propagation in the cavity is characterized by the acoustic inhomogeneous wave equation written in terms of the velocity potential. The actuating forces of the piezoelectric patches due to control are expressed by equivalent bending moments. The control loop is closed by different feedback algorithms like velocity feedback control and optimal linear quadratic control.

For solving the coupled equations, a modal approach is used, in which the unknown field variable, i.e. velocity potential and the plate displacement, are approximated as a sum of the uncoupled acoustic modes and structural modes. The analytical solution is compared with numerical simulations as well as experimental data from measurements.

Modelling wave-propagation phenomena in time domain using the symmetric Galerkin BEM and convolution quadrature method.
Lars Kielhorn Kielhorn (Universität Graz, Austria), Martin Schanz (TU Graz, Austria) GA/CT2703/012

The understanding and modelling of wave propagation phenomena are of great importance in many engineering applications. Those phenomena can be effectively analyzed with the Boundary Element Method (BEM), especially in large or unbounded media. Nowadays in engineering, the spatial discretization of the underlying time-dependent Boundary Integral Equations (BIEs) is mostly done via the Collocation method. For the time discretization the Convolution Quadrature Method (CQM) proposed by Lubich is considered. This time stepping procedure is based only on the fundamental solutions in Laplace domain and, therefore, can also deal with problems where the fundamental solutions are not available in time domain.

The present work focuses on time-dependent BIEs arising from elastodynamics and the scalar wave equation. Again, the chosen time stepping procedure is the CQM but instead using a collocation method, a variational formulation is used resulting in a Galerkin based method in space. As will be shown numerically, this kind of discretization leads to an improvement of the numerical stability with respect to the time discretization.

In almost all engineering applications, mixed boundary value problems have to be solved, i.e., not only pure Dirichlet or pure Neumann problems are under considerations. Therefore, additionally to the 1st BIE also the 2nd BIE is used. Evaluating the 1st BIE on the Dirichlet part of the boundary and the 2nd BIE on the Neumann part of the boundary leads, finally, to a skew-symmetric linear system of equations, which may has better solution properties than those systems obtained by standard collocation methods.

After a short discussion of some necessary implementation details, both methods, the proposed Galerkin approach using the 1st and the 2nd integral equation and the more common Collocation approach using only the 1st integral equation, are compared with respect to the spatial and temporal discretization.

On the automated generation of reduced-order models in flexible multibody dynamics. **Jörg Fehr** (ITM, University of Stuttgart, Germany), Michael Lehner (Universität Stuttgart, Germany), Peter Eberhard (Universität Stuttgart, Germany) GA/CT1962/012

An important issue in the field of flexible multibody dynamics is the reduction of the flexible body's degrees of freedom. In this regard, a classical method is modal reduction. However, as the spatial character of the load acting on the body is not taken into account, convergence can be very slow. To improve convergence, the eigenvectors are often supplemented with additional assumed modes, e.g, static modes or frequency response modes. However, the choice of the proper set of basis vectors, consisting of eigenmodes and assumed modes, is a crucial task that requires much experience and insight into the specific problem. By the use of Gramian matrix based reduction techniques the distribution of the loads is taken into account *a priori*. Furthermore, an energy interpretation of the reduction procedure and error bounds in the frequency domain are available. In this work a frequency weighted second order Gramian matrix is defined that allows to generate a very accurate approximation of the flexible body's transfer function in a predefined range of the spectrum. Also, the stability properties of the original system are preserved. Hence, using this method only the load distribution, the frequency range of interest and a measure for the desired accuracy has to be provided. For diagonalizable models the second order Gramian matrix can be calculated analytically. However, appropriate approximation schemes have to be developed for large scale models. Here, we introduce such methods and discuss the convergence properties and suitable stopping criteria. The goal of the work is to provide a fully automated reduction process for flexible substructures in multibody systems. A numerical example demonstrates the approximation capability of the proposed technique in the frequency and time domain.

An Euler-solver for the acoustic far-field prediction of compressible jet flow. **Felix Keiderling** (ETH Zürich, Switzerland), Dominik Obrist (ETH Zürich, Switzerland), Sebastian Müller (ETH Zürich, Switzerland), Leonhard Kleiser (ETH Zürich, Switzerland) GA/CT2442/012

We report on a high-accuracy Euler solver developed for far-field jet noise prediction. The code is embedded in a framework of a Direct Numerical Simulation (DNS) / Large-Eddy Simulation (LES) code [1] providing the time-dependent, noise-generating flow field and the acoustic near-field.

The motivation for this development is twofold: First, we would like to efficiently and accurately predict jet noise not only in the acoustic near-field but also in the far-field region which is subject of most experimental investigations, as well as of interest to most practical applications. Second, we want to investigate the operative range of a previously developed analytical acoustic far-field solver, the SLM (Spectral Lighthill method), which is based on Lighthill's acoustic analogy [2].

The Euler solver employs the conservative formulation of the governing equations in generalized coordinates (ξ, η, ζ) that are mapped to a cylindrical frame of reference (r, θ, z). The set of equations is discretized using the same numerical components as the DNS/LES code, i.e., a highly accurate spatial discretization (with spectral-like resolution properties of $6th$ to $10th$ order compact-finite differences in the radial and streamwise directions and a Fourier spectral method in the azimuthal direction) combined with a fourth-order Runge-Kutta scheme in time that is optimized with respect to its dispersion and dissipation properties [3]. Numerical stability is ensured by employing the ADM-RT (relaxation-term) subgrid-scale closure developed within our group.

Details of the computational scheme will be presented. Results of the validation will be shown along with a comparison between predictions of the Euler solver and the SLM for analytical test cases.

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[2] D. Obrist, F. Keiderling, and L. Kleiser. Computation of acoustic far-fields with the Spectral Lighthill Method. *Proc. Appl. Math. Mech.*, 2006.

[3] J. Berland, Ch. Bogey, and Ch. Bailly. Low-dissipation and low-dispersion fourth-order Runge–Kutta algorithm. *Comput. Fluids*, 35:1459–1463, 2006.

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GA/CTS4869/13: **Mechanical systems and robotics.**

Organiser: Peter Eberhard (Universität Stuttgart, Germany)
Co-organiser: Uwe Helmke (Julius-Maximilians-Universität Würzburg, Germany)

Dynamisches Positionieren eines schwimmenden Körpers. **Marc-André Pick** (TU Hamburg-Harburg, Germany), Edwin Kreuzer (TU Hamburg-Harburg, Germany), Jörg Wagner (Universität Stuttgart, Germany) GA/CT1501/013

Numerische Bifurkationsuntersuchungen haben gezeigt, dass das Kentern von Schiffen durch eine Sequenz von Verzweigungen in der Dynamik des Systems "Schiff im Seegang" beschrieben werden kann. Um die Analyse zu beschleunigen, soll das verwendete und weltweit anerkannte nichtlineare Modell zur Beschreibung der dreidimensionalen Schiffsbewegung einschliesslich der Fluid-Struktur-Wechselwirkung durch reduziert werden. Zur Validierung der Modellreduktion ist es nötig, reproduzierbare Versuche mit einem schwimmenden Testkörper einfacher Geometrie unter genau definierten Bedingungen wiederholt durchzuführen. Zu diesem Zweck wurde ein dynamisch positionierbarer Schwimmkörper entwickelt, mit dem diese Forderungen im Wellenkanal des Institutes erfüllt werden können. Dabei ist es möglich, in einem frei zur Welle wählbaren Winkel die Antwort des Körpers auf die anregenden Wellen zu messen. Der Schwimmkörper ist mit sechs Aktoren (Waterjets) ausgestattet, die Schub in jeweils eine Richtung liefern. Es lassen sich damit die drei Freiheitsgrade ohne hydrostatische Rückstellkraft (Vorwärts-, Drift- und Gierbewegung) ausgleichen. Die Bestimmung von Position und Lage des Körpers wird durch ein integriertes Messsystem erreicht, das aus einer Stereo-CCD-Kamera und einer inertialen Messeinheit, die Beschleunigungen und Winkelgeschwindigkeiten bezüglich der körperfesten Achsen misst, besteht. Über ein erweitertes Kalman-Filter werden die beiden Messsysteme miteinander kombiniert, indem die Drift der Inertialmessung (Abtastperiode 5ms) durch Vergleich mit der durch die Kamera gemessenen Position (Abtastperiode 100ms) kompensiert wird. Damit werden langzeitstabile Messungen mit hoher Dynamik durchgeführt, die dem Regler als Rückführung dienen, und die für weitere Analysen aufgezeichnet werden.

Optimal design of a 2 DOF parallel robot. **Sergiu-Dan Stan** (Universitatea Tehnicã Cluj-Napoca, Romania) GA/CT92/013

The aim of this paper is to show the usefulness of the multicriteria approach to optimize the parallel robots. Variations of the kinematic performances index remain not constant throughout workspace. The potential of parallel robots is only then efficient exploited when their structure is optimal dimensioned from geometric point of view. So, their performances depend very strong on their geometry. Thus, optimization of the geometric parameters or optimal dimensioning has become an important issue for improving the parallel robots performances. Aiming to deal at the same time with multiple criteria in optimal design of parallel robots, we have developed a multiobjective genetic algorithm (MOGA) using concepts of Pareto optimality and niching techniques. Here, intended to show the advantages of using the MOGA, we applied it to a multicriteria optimization problem of 2 dof parallel robot. Genetic algorithms (GA) are so far generally the best and most robust kind of evolutionary algorithms. A GA has a number of advantages. It can quickly scan a vast solution set. Bad proposals do not affect the end solution negatively as they are simply discarded. The obtained results have shown that the use of MOGA in such kind of optimization problem enhances the quality of the optimization outcome, providing a better and more realistic support for the decision maker.

Force control of a fluidic-muscle-driven parallel platform. **Mahendra Dhanu Singh** (Universität Duisburg-Essen, Germany), Kusnadi Liem (Universität Duisburg-Essen, Germany), Rüdiger Neumann (Festo AG & Co. KG, Germany), Andres Kecskemethy (Universität Duisburg-Essen, Germany) GA/CT2255/013

In this paper a force control scheme for a parallel platform consisting of six fluidic-muscle actuator legs of type RRPS is presented. The objective of the control algorithm is to emulate arbitrary variable 6×6 stiffness properties at the end effector, such as needed for example to physically simulate soft tissue for component-in.the.loop testing. Fluidic muscles are well suited as actuators in robotics, since they have a high power/weight ratio, long durability and slip-stick-free motion. On the other hand, fluidic muscles require that the gas model as well as the rubber nonlinearities are included in the control scheme. Moreover, the control law for the gas flow in the proportional directional control valve in 3/3-way function needs to be taken into account. The present paper describes the basic dynamic models as well as testbed results for the existing fluidic-muscle parallel platform "HexaSpine", here each leg is equipped with a force sensor, a pressure sensor and a magnetostrictive position encoder respectively. The control scheme for the platform comprises six control loops for the six operated actuators with a model based force control each. It is shown that the aforementioned control scheme leads to a rapid stiffness simulation. As an application, the device will be employed in fields of biomechanics for physical simulation of cervical-spine motion, as well as in general environments requiring soft tissue physical simulation.

A method for determining control inputs for prescribed accelerations of the end-effector of an industrial robot. **Martin Tändl** (Universität Duisburg-Essen, Germany), Andres Kecskemethy (Universität Duisburg-Essen, Germany) GA/CT2721/013

Described in this paper is an approach for generating control inputs for an industrial Kuka robot such that it produces prescribed linear acceleration time histories for a given point of the end-effector. The method takes into account the workspace limits, and uses the internal interpolation cycle of the robot controller to generate the corresponding trajectories that will produce the prescribed accelerations. The PID parameters of the internal interpolation are identified from test measurements. The control scheme consists in producing time-varying values for the desired angle values of the interpolation algorithm, making the changes as the algorithm proceeds and thus generating smooth trajectories. The resulting acceleration of these trajectories is compared to the prescribed accelerations, and an optimization procedure is run such as to determine the required time-histories of the desired angles for the interpolation algorithm such that both accelerations match. The approach is demonstrated for the example of a 500kg payload Kuka robot that is aimed at producing given motions as a physical motion simulator (e. g. for cars or complex working machines). It is shown that the desired accelerations can be generated accurately and with high repeatability, making the approach suitable for example for simulating car rollover tests.

The Hide-Skeldon-Acheson dynamo revisited. **Irene Moroz** (University of Oxford, UK) GA/CT4375/013

Hide et al (1996) introduced a nonlinear system of three coupled ordinary differential equations to model a self-exciting Faraday disk homopolar dynamo. A very small selection of its possible behaviours was presented in that paper. Subsequent studies have extended the system to incorporate the effects of a nonlinear motor, an external battery and magnetic field, the coupling of two or more identical dynamos together, amongst other things. In this talk we return to the original model with a view to performing a more extensive analysis of the Hide et al (1996) dynamo. For the first time we present bifurcation transition diagrams, so that the two examples of chaotic dynamo action shown as figure 9 in that paper can now be placed into context. We exhibit the coexistence of multiple attractors and also identify the lowest order unstable periodic orbits pertaining to some specific cases.

GA/CTS4870/13: Vibration control and damping.

Organiser: Uwe Helmke (Julius-Maximilians-Universität Würzburg, Germany)
Co-organiser: Peter Eberhard (Universität Stuttgart, Germany)

Vibration elimination in cable-stayed footbridges and bridges. **Wojciech Pakos** (Wroclaw University, Poland), Zbigniew Wójcicki (Wroclaw University of Technology, Poland), Jacek Grosel (Wroclaw University, Poland) GA/CT3023/013

In this paper, the problems of eliminating vibration in cable stayed footbridges and bridges by dynamically steering the tension in cables during construction vibration are considered. A physical and a mathematical model of cable stayed footbridges and bridges has been formulated. A damping model has been selected on the basis of an analysis of vibrations due to periodic excitation. Standard computer software and the authorŠs own program, both leaning on Finite Element Method (FEM), have been used to analyze the eigenproblem and the forced vibration of bridges. On the basis of the formulated theory an efficient algorithm of forced vibration reduction analysis was established. The reduction is achieved by dynamically steering the tension in cables. A sensitivity analysis has been used. An example has been provided. The theory presented takes into account the new method in the elimination of vibration in cable stayed bridges and footbridges. It can therefore be applied to dynamic analysis of modern cable stayed bridges with typical structure systems.

Active control of working machines seat suspension aimed at health protection against vibration. **Igor Maciejewski** (Koszalin University of Technology, Poland) GA/CT3092/013

The paper presents the model and simulation of passive and active earth-moving machines seat suspension. The object of the simulation is the visco-elastic passive seat suspension with an air-spring, hydraulic shock-absorber and scissors guidance mechanism. Based on the measurements of the passive seat, the stiffness, damping coefficient and friction force is evaluated in this way, that the behavior of real seat suspension and model is nearly the same. Passive seat suspension amplifies the vibration amplitude at low frequency range of excitation signal (the resonance effect). The lowest resonance frequencies of human body parts occur for the internal organs of abdominal cavity (stomach: 2-3 Hz). In order to help the working machines operators against vibration, the active system with different control strategies is elaborated. Active system improves significantly the behavior of the seat suspension at low frequency excitation, with the most effectiveness obtained for the resonance frequency. The simulation is carried out using the excitations in accordance to ISO 7096 standard. As the results of the computer simulation, the power spectral densities of acceleration for a seat is presented in comparison with sample excitations on the earth-moving machines cabin floor. Additionally, the transmissibility functions for a passive suspension and the corresponding active suspension are shown.

Voltage-amplification transfer-function analysis of the operational amplifier in the negative-capacitance circuits for vibration control with piezo-ceramics. **Robert Oleskiewicz** (Koszalin University of Technology, Poland), Marcus Neubauer (Universität Hannover, Germany), Tomasz Krzyzynski (Koszalin University of Technology, Poland) GA/CT2787/013

Piezo elements due to their ability of converting mechanical energy into electrical energy and vice versa can be found in numerous mechanical vibration damping and absorbing applications. A desired effect may be customized by an external impedance shunt branch connected to the plates of the piezo element. The recent research shows that the negative capacitance connected in serial with the passive shunt significantly improves the damping and absorbing performance of such systems. Negative capacitance circuit is built up of an electronic impedance converter realized by the operational amplifier. Since the operational amplifiers are not the ideal elements, the performance of the proposed systems is limited, especially for small values of the electromechanical coupling coefficient of the piezoceramics. The main limitation, beside the maximum voltages and currents at which the operational amplifiers operate, comes from the finite gain of the circuit and the phase lag between the input and the output terminals. This effect causes instabilities and limits the operational area of the impedance converter. In the paper, the amplification transfer function of the non-ideal operational amplifier in the negative impedance converter is studied, and the necessary modification with the additional passive elements is proposed. The influence of the certain imperfections in the design, and its improvements are shown on the system consisting of the 1DOF mechanical oscillator, and a shunted piezo element.

Modeling of a vehicle seat suspension system with pneumatic spring and viscous dampers. **Sebastian Chamera** (Koszalin University of Technology, Poland), Igor Maciejewski (Koszalin University of Technology, Poland), Tomasz Krzyzynski (Koszalin University of Technology, Poland) GA/CT3035/013

The paper contains physical and mathematical model of the passive system of seat suspension, used in trucks and buses. The object of modeling is the Czech made serial produced seat. Spring force in this system is performed by air spring, whereas damping force is generated in two viscous dampers. Based on the experimental research of characteristic parts of the suspension system, the parameters of mathematical model are determined. Simulations and experiments are done by using white noise excitation in frequency range of 0-10 Hz, and two different excitations, according to ISO 7096. Both results of computer simulations and experiments are presented as power spectral density of acceleration courses, measured on seat, in comparison with courses measured on excitation platform in laboratory. Transmissibility of real system and its model are also presented in the paper. To estimate vibroisolation properties, SEAT (Seat Effective Amplitude Transmissibility) factor is determined, according to the standard, estimated at weighted values of frequencies. Given results enable further improvement of suspension system and better vibroisolation properties.

Method for evaluation of movement resistance in Scarper pipe conveyors. **Kazimierz Furmanik** (University of Science and Technology, Poland), Michal Pracik (Cracow University of Technology, Poland) GA/CT2163/013

Scarper pipe conveyors find more and more broad use in transportation of loose and powdery materials because this mode of material transport remains a cost-effective method. One can point disadvantages of these conveyors - a relatively large movement resistance inside the pipe, especially on vertical routes, and abrasive wear of chutes and chains. The state of art in designing of such conveyors is still not satisfactory. Rational process of designing needs a new approach to estimation of movement resistance, which will take into account basic parameters of conveyor construction and properties of transported materials. In the paper there is introduced a new method of determination of movement resistance and presented experimental verification basing on results of investigations carried out on a suitable stand up. Using the method one can perform a variety of calculations of the conveyor construction in order to find optimum values of its parameters that meet required capability, capacity and lower horsepower consumption. Analysis of theoretical and experimental investigation results related to the proposed method let formulate final conclusions.

Stability constraints in optimization of cracked columns subjected to compressive follower load. **Szymon Imielowski** (Institute of Fundamental Technological Research, Poland), Roman Bogacz (Institute of Fundamental Technological Research, Poland) GA/CT4250/013

Maximization of the critical force of cracked columns, subjected to generalized follower load is considered. In the modern mechanical structures the follower force can be caused; e.g., by systems of active control. The crack is assumed to be formed according to the opening and sliding modes and is modeled by localized loss of stiffness namely by elastic joint with possible rotational and shear deformation. The column is modeled by Bernoulli–Euler beam. The equation of motion for small harmonic vibration of are taken into consideration.

The crack localization and its stiffness which maximizes the critical load under the constraints of a constant total column mass and length and a constant column cross-sections are developed. The objective function $\lambda^*_{\mathrm{cr}} = \lambda^*_{\mathrm{cr}}(\Delta\alpha)$, where $\Delta\alpha$ stands for a set of design variables, is not defined explicitly. The optimization conditions, imposed in the frequency domain, are defined as limitations on variation of the shape of characteristic curves. The optimal point is defined as one that represents the state for which all pairs of eigencurves become double roots with the same value of critical forces. In the multimodal analysis the first six eigenfrequencies are considered.

An influence of the crack stiffnesses and its localization on the value of the critical force is presented. The localization of crack with the critical force of the system equal to $137.17\,\mathrm{EJ/L^2}$ is found.

GA/CTS4866/13: System and control theory, I.

Organiser: Uwe Helmke (Julius-Maximilians-Universität Würzburg, Germany)
Co-organiser: Peter Eberhard (Universität Stuttgart, Germany)

Computing minimal optimization horizons for stabilizing unconstrained MPC schemes. **Lars Grüne** (Universität Bayreuth, Germany) GA/CT1544/013

In this talk we consider MPC schemes for nonlinear discrete time systems in arbitrary metric spaces. More precisely, we consider the MPC feedback law $F(x_0) := u_0$ obtained from the online solution of the finite horizon optimal control problem

$$\min_{u_0,\ldots,u_{N-1}} \sum_{j=0}^{N-1} \ell(x_j, u_j)$$

where x_j, $j = 0, 1, \ldots$, denotes the system trajectory for initial value x_0 and control sequence $u_0, \ldots, u_{N-1}$. If the system is exponentially controllable to the origin and the running cost $\ell(x, u)$ is a positive definite function in x, then it is well known that the resulting feedback F stabilizes the closed loop for sufficiently large (but in general unknown) optimization horizon N.

In this talk we assume null-controllability of $\ell(x_j, u_j)$ with prescribed bounds on the attraction rate and overshoot, and look for the minimal optimization horizon N^* for which asymptotic stability of the closed loop holds. Minimal here is to be understood in the sense that for any optimization horizon $N < N^*$ there exists a system which satisfies the assumed controllability property and is not stabilized by the MPC feedback law with this N.

We show that if the assumed controllability property is linear in the initial value (as, e.g., for exponential controllability or for finite time controllability with linear bound on the overshoot), then this problem can be formulated as a linear program whose complexity is independent on the dimension of the state space and on the degree of nonlinearity of the underlying dynamics. This linear program is of moderate complexity and can thus be solved by standard solvers. Based on the numerical findings from this procedure we are then able to conjecture on theoretical bounds for the optimal N^* depending on overshoot and attraction rates.

A min–max version of Dijkstra's algorithm with application to perturbed optimal control problems. **Marcus von Lossow** (Universität Bayreuth, Germany), Lars Grüne (Universität Bayreuth, Germany), Oliver Junge (TU München, Germany) GA/CT1757/013

Discrete time optimal control problems over an infinite horizon are studied for themselves or are obtained by a time-discretization of a continuous time control system. Perturbed systems of that kind are often used to describe mechanical or economic problems subject to external perturbations. On the other hand, the error caused by the numerical state-space-discretization of an unperturbed system can also be considered as a perturbation of the system.

In our talk we present a new method for solving this kind of problem. The method is based on a set oriented discretization of the state space in combination with a new algorithm for the computation of shortest paths in weighted directed hypergraphs. One of the fastest algorithms for shortest path problems, Dijkstra's algorithm, can be extended to a "min-max Dijkstra" algorithm. We will describe this algorithm and discuss suitable data structures and the corresponding computational complexity which increases only moderately using a suitable implementation. Furthermore we will give an outlook on how to use this approach to construct a suboptimal feedback to stabilize such control systems.

This new approach will be illustrated by a number of numerical examples.

Minimum-time optimal interception with terminal constraints. **Vasile Istratie** (National Institute for Aerospace Research, Romania) GA/CT2112/013

This work studies the interception laws for maneuvering targets with known trajectories in the of the three-dimensional in case minimum time optimal, while in Ref. 1 and 2, where this problem is solved for the minimum of fuel. Optimal interception problems are defined, which include constraints on final flight-path angles of the interceptor. The interceptor is moving at a constant velocity and can change its flight direction by applying bounded normal acceleration. The variational problem is of Mayer (or Lagrange) type, and the optimum control to be determined being angles acceleration direction The target is moving along an *a priori* known trajectory with known velocity. The coordinates describe the location of the interceptor and the target, respectively, relative to the origin of an arbitrary reference coordinate system. The problem is to find the angles acceleration direction - the optimal control input time history, so that the equations of the interceptor are satisfied and the performance index (the minimum time) is minimized while intercepting a target with a known trajectory. By means of the Legendre-Clebsch condition it is demonstrated that the formulated optimization problem is a maximum problem. The optimization problem is solved applying the PontriaghinŠs maximum principle, as well as in the problem from Ref. 1-3. So, the above defined problem of optimal control is transformed in a two point boundary problem. The nonlinear differential equations of the extremes where any kind of approximation was eliminated are precisely integrated by a numerical method, shooting, [4], [5]. Numerical examples that demonstrate the optimal trajectories are presented showing also the effect of the interceptor final flight-path angles on the interception characteristics.

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A note on the numerical treatment of dynamical systems with friction. **Alexander Lünenschloß** (TU Darmstadt, Germany) GA/CT3175/013

The modeling of dynamical systems with friction leads to ODEs with discontinuous right-hand side. In this case the phase space contains manifolds where the directions of the crossing trajectories are discontinuous. In regions of these manifolds trajectories may point towards each other, and the solution stays on the manifold. This behavior is called sliding mode, but it is not covered by classical theory of ODEs. The regularization of the discontinuities leads to solutions that show undesired properties. A numerical computation based on Filippov's sliding-mode definition shows the desired behavior: In this case the time of a complete trajectory can be composed of intervals alternating classical solutions and sliding modes. These alternating intervals require different algorithms, and so does the transition between them. The given examples compare regularized and compound solutions.

Optimal singular control for systems involving parameters. **Mihai-Emilian Popescu** (ISMMA-Bucharest, Romania) GA/CT3143/013

What we shall take into consideration is represented by the problems of singular optimal control when the index of performance, the differential constraints and the final conditions contain parameters. What is determined is the trajectory of the neighboring extremal for the initial point perturbed at the constraints of the perturbed final manifold. The present study evaluates the variation of the command on the extremal. This one allows obtaining the second variation in the singular case. The sufficient conditions of minimum are a result of imposing the non-negativity of the second variation. The application made analyses the optimality of the singular control for a system in the class of affine differential systems.

A variational approach to optimal control problems for elastic body motions. **Georgy Kostin** (Institute for Problems in Mechanics RAS, Russian Federation), Vasily Saurin (Institute for Problems in Mechanics RAS, Russian Federation) GA/CT809/013

The initial-boundary problem for the linear theory of elasticity is considered. Based on the method of integrodifferential relations a new dynamical variational principle in which displacement, stress, and momentum functions are varied is proposed and discussed. To minimize the nonnegative functional under initial, boundary, and differential constraints arising in this approach a regular algorithm for approximation of the unknown functions is worked out. The algorithm gives us the possibility to estimate explicitly the local and integral quality of obtained numerical solutions. An effective numerical method for the optimization problems of controlled motions of elastic bodies with quadratic objective functionals is developed. As example, the 3D problems of optimal longitudinal motions of a rectilinear elastic prism with a quadratic cross section are considered for the terminal total mechanical energy to be minimized. The numerical results and their error estimates are presented and discussed.

GA/CTS4867/13: System and control theory, II.

Organiser: Uwe Helmke (Julius-Maximilians-Universität Würzburg, Germany)
Co-organiser: Peter Eberhard (Universität Stuttgart, Germany)

Practical tracking with prescribed behaviour for electric drives. **Achim Ilchmann** (TU Ilmenau, Germany) GA/CT1819/013

We consider a two-mass flexible servo system with flexible connection between machine and load modelled, see for example [2], by

$$\dot{x}(t) = A\,x(t) + b\,u(t) + b_T\,\psi(\omega_2(t))\,, \qquad (1)$$

with

$$A = \begin{bmatrix} -d/J_2 & k/J_2 & d/J_2 \\ -1 & 0 & 1 \\ d/J_1 & -k/J_1 & -d/J_1 \end{bmatrix}, \quad b = \begin{pmatrix} 0 \\ 0 \\ 1/J_1 \end{pmatrix}, \quad b_T = \begin{pmatrix} -1/J_2 \\ 0 \\ 0 \end{pmatrix},$$

where the state vector $x = (\omega_2,\ \Delta\varphi,\ \omega_1)^T$ contains the speed of the load, the angle of twist between the drive and the load and the speed of the drive, $\psi\colon \mathbb{R} \to \mathbb{R}$ models the nonlinear friction force depending on ω_2 and is assumed to be bounded with unknown bound.

A prototypical example for the model is an electric drive. In industrial applications induction machines are used which are supplied by an AC-converter. Since the underlying current control loop is based on the speed of the drive, a sensor for ω_1 is indispensable. The controlled variable ω_2 is assumed to be measurable as well. These two variable allow for a reduction of the relative degree. Without measurement of the angle of twist no active damping can be provided by a PI-controller,

even if the plant is perfectly known [2]. Hence a sensor for $\Delta\varphi$ is import for good performance. In some applications position sensors are used such that the state $\Delta\varphi$ is computed very easily by a simple difference of the position of both masses. Thus we consider an output y so that the system $u \to y$ has relative degree one.

Next we show that the zero dynamics are asymptotically stable; this global result is an extension of local results[3].

Moreover, rewriting the system in an appropriate form it can be shown that it belongs to the class of systems that have been studied[1], so that *funnel control* is applicable. A funnel controller ensures that the error between the output of the system and a reference signal, $e = y - y_{\mathrm{ref}}$, evolves within a prespecified *funnel*. This controller is simple in its design, it is a sort of adaptive controller, not based on any identification mechanisms.

The theoretical results are underlined by experiments with a two-mass flexible servo system. The obtained results show, that the presented control strategy is appropriate for electrical drive systems in industrial applications.

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An adaptive fuzzy controller for nonlinear systems with dead-zone. **Wallace Bessa** (Centro Federal de Educação Tecnológica, Brazil), Max Dutra (Universidade Federal do Rio de Janeiro, Brazil), Edwin Kreuzer (TU Hamburg–Harburg, Germany) GA/CT2777/013

The dead-zone nonlinearity is frequently encountered in many physical components of industrial control systems, especially those containing some very common actuators, such as hydraulic proportional valves and electric motors. Dead-zones are often poorly known and their characteristics may also vary with time. It was already observed that their presence can severely reduce control system performance and lead to limit cycles in the closed-loop system. Due to the possibility to express human experience in an algorithmic manner, fuzzy logic has been largely employed in the last decades to both control and identification of uncertain dynamical systems. In spite of the simplicity of this heuristic approach, in some situations a more rigorous mathematical treatment of the problem is required. Our aim is to present an adaptive fuzzy control scheme for nonlinear systems with unknown dead-zone. The stability properties of the closed-loop system will be proven using Lyapunov stability theory and Barbalat's lemma. Numerical results will be also presented in order to demonstrate the control system performance.

Cell-mapping methods for random dynamical systems. **Andreas Gaull** (TU Hamburg–Harburg, Germany), Edwin Kreuzer (TU Hamburg–Harburg, Germany) GA/CT1551/013

This contribution is concerned with the numerical study of the global behavior of dynamical systems subjected to stochastic perturbations. An extended version of the Cell Mapping method is employed as a numerical toolbox.

For deterministic systems, Cell Mapping represents an approximation of the Frobenius–Perron operator by a Galerkin method. This operator describes the evolution of densities under a given system transformation. We want to point out how this concept can be expanded to Random Dynamical Systems and specify a stochastic analog of the deterministic Frobenius–Perron operator. The method of Cell Mapping provides finite dimensional approximations of invariant densities and allows a characterization of attractors as well as the basins of attractions. At this juncture, investigation of the discretized Frobenius–Perron operator is based on the techniques from symbolic dynamics.

Optimal control of structure-variant rigid-body mechanical systems. **Kerim Yunt** (ETH Zürich, Switzerland) GA/CT1024/013

A measure differential inclusion (MDI) based modeling approach for rigid-body mechanical systems will be introduced, that can exhibit autonomous or controlled mode transitions, accompanied by discontinuities on velocity and acceleration level. The introduced framework will have the ability to model and control of hybrid mechanical systems with discontinuous transitions among different system modes. Modeling of rigid-body Lagrangian systems as LCP will be presented. The properties of the optimal control problem derive from the underlying modeling approach. The main issue in the optimal control of hybrid mechanical systems has been the blending of impact mechanics with impulsive optimal control. The discontinuities arising from impacts and stick-slip transitions are primarily contact phenomena, which conccure temporally and spatially. The spatial conccurence of discontinuity is due to the fact that discontinuities on velocity level (e.g. collisions) can occur along with discontinuities on acceleration level (e.g.stick-slip transitions). Temporal conccurence is caused by collision, shock and impact phenomena occuring at multiple locations of the system at the same time as well as stick-slip transitions. Recent research showed that such rigid-body systems can best be described by variational inequalities which lead to nonlinear and linear complementarity type of systems to be solved in order to obtain the accelerations/velocities and forces. In the modeling considered in this work, impulsive forces can arise autonomously, due to effects such as collisions or controlled/nonautonomously, due to actions such blocking some DOF. The hybrid optimal control requires the consideration of an uncommon concept of control, namely, controls of unbounded, impulsive and set-valued type.

Minimum integrated altitude control for the terminal bunt manoeuvre. **Subchan Subchan** (Cranfield University, UK) GA/CT3014/013

An optimal control problem of a generic cruise missile attacking a fixed target in minimum altitude along the trajectory is investigated. The missile must struck the target from above, subject to missile dynamics and path constraints. The generic shape of the optimal trajectory is: level flight, climbing, diving; this combination of the three flight phases is called the bunt manoeuvre. The numerical solution of optimal control problem is solved by combination of a direct method and an indirect method. A direct approach based on a collocation method is used to reveal the structure of the optimal solution which is composed of several arcs, each of which can be identified by the corresponding manoeuvre executed and constraints active. The direct approach produces approximate solutions for both states and co-states. The indirect approach is then employed to derive optimality conditions based on Pontryagin's Minimum Principle.

Generalized p-Galerkin time-integration schemes for durability mechanics and structural dynamics. **Detlef Kuhl** (Ruhr-Universität Bochum, Germany) GA/CT3558/013

The present paper is concerned with generalized discontinuous and continuous Galerkin time integration schemes of arbitrary polynomial degree (dG(p) and dG(p)) to single- and multifield structural mechanics. In particular, first order semidiscrete initial value problems associated with transport dominated computational durability analyses described by the non-linear vector differential equation $\mathbf{r}_i(\dot{\mathbf{u}}, \mathbf{u}) = \mathbf{r}(t)$ and second order semidiscrete initial value problems associated with computational structural dynamics $\mathbf{r}_i(\ddot{\mathbf{u}}, \dot{\mathbf{u}}, \mathbf{u}) = \mathbf{r}(t)$ are solved by this class of algorithms. Therefore, the discontinuous GALERKIN schemes proposed by [1,2] and the continuous GALERKIN schemes proposed by [3,4,5] are formulated within a generalized framework. This family of p-GALERKIN time integration schemes includes the numerically dissipative and energy conserving continuous Galerkin schemes as well as the discontinuous GALERKIN method for first and second order nonlinear problems as special cases. Studies of discontinuous and continuous GALERKIN schemes in the context of calcium leaching of cementitious materials shows the potential of this integration methods in the presence of non-smooth DIRICHLET boundary conditions, non-smooth initial conditions and moving dissolution fronts. Furthermore, the order of accuracy of dG(p)- and cG(p)-schemes can be controlled by the polynomial degree $\mathcal{O}(p)$ and $\mathcal{O}(p+1)$, respectively. The application of discontinuous GALERKIN schemes to non-linear structural dynamics illustrates the stable numerical solution, the dissipation of energy within the high frequency range of the structural response and the controllable higher order of accuracy $\mathcal{O}(2p+1)$. Depending on the damping parameter [5], $2p$th order accurate generalized continuous GALERKIN schemes cG(p) applied to HAMILTONian systems are characterized by the conservation or decay of total energy.

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GA/CTS4868/13: System and control theory, III.

Organiser: Uwe Helmke (Julius-Maximilians-Universität Würzburg, Germany)
Co-organiser: Peter Eberhard (Universität Stuttgart, Germany)

Model reduction for bilinear diffusion and diffusion–reaction systems. **Tobias Damm** (TU Kaiserslautern, Germany), Peter Benner (TU Chemnitz, Germany) GA/CT3071/013

Discretization of diffusion equations with Neumann-type boundary control or reaction-diffusion equations leads to large-scale bilinear control systems of the form

$$\dot{x} = Ax + \sum_{j=1}^{k} N_j x u_j + Bu\,, \quad \text{with} \quad y = Cx\,.$$

In some respects these systems still behave like linear systems. For instance, if A is stable, then the system defines a bounded input/output operator $G : L^2 \to L^2$ by setting $Gu = y$. Therefore, it is natural to look for an approximation of G by an input/output operator G_r of a lower dimensional system.

One simple, but easy to implement approach is to use the state-space projections obtained by balanced truncation (based on the Gramians) of the linear part of the system (with $N_j = 0$), and apply these projections to the bilinear system. A more advanced idea is to obtain the projections by balancing generalized Gramians of the bilinear system. For selected examples, we compare these approaches with respect to their computational complexity and the error $\|G_r - G\|$.

Constraints on the convergence behaviour of algorithms via reachable set analysis. **Jens Jordan** (Universität Würzburg, Germany) GA/CT2670/013

Many iterative algorithms can be interpreted as discrete-time control systems evolving on manifolds. Here, shift parameters act as control inputs. The Adherence structure of the reachable sets provides fundamental limitations on the possible convergence behaviour of the algorithm.

We analyse the reachable sets and their structure for a family of numerical algorithms, using geometric and algebraic tools. We apply our results on well-known numerical algorithms, such as Inverse Iteration and Richardson Iteration. In particular, we show necessary conditions for the existence of local convergent shift strategies and feedback laws.

Dynamics of open quantum systems. **Uwe Helmke** (Julius-Maximilians-Universität Würzburg, Germany), Gunther Dirr (Julius-Maximilians-Universität Würzburg, Germany), Indra Kurniawan (Universität Würzburg, Germany) GA/CT2181/013

The dynamics of open quantum systems is desribed by the Lindblad equation on positive-semidefinite Hermitian operators. As shown by Lindblad (1976) using functional analytic methods, the differential equation preserves the class of completely positive operators. In this talk we present an approach based on the theory of Lie semigroups to tackle this problem, in particular concerning preservation of positive semidefiniteness under the flow. We also discuss some problems concerning controllability of a two spin system.

Actuated conformation change in a chain of oscillators. **Philip Du Toit** (California Institute of Technology, USA) GA/CT2843/013

We study robustness and control in a system of coupled oscillators that exhibits two conformational states. Each conformation is robust against large random perturbations, yet the action of a small structured perturbation that excites resonances in the natural dynamics of the oscillator chain causes the chain to coherently and robustly undergo a conformation change from one state to the other. Therefore, the oscillator chain has the interesting property that it remains locked in a conformational state for large random perturbations, but global conformational change can be easily induced by the action of a small targeted control. Our motivation for studying this oscillator chain arises in the study of biopolymers that exhibit exactly this property. DNA, for instance, is well-known to be a stable biomolecule requiring temperatures in excess of $60°$C to induce melting or denaturalization of the DNA helix, yet specialized proteins such as helicase and polymerase are able to robustly unlock the DNA strands and induce melting so that the essential processes of DNA replication and transcrip-

tion can occur.

More specifically, we consider a class of biopolymers that can be modeled as a chain of pendula attached to a rigid backbone. The motion of each pendulum is governed by two interactions: each pendulum interacts with its nearest neighbor through a harmonic potential that models torsional coupling through the backbone, and secondly, each pendulum moves in a Morse potential that models the weaker Hydrogen bonding interaction between pendulum pairs on a complementary chain. We observe that the Morse potential establishes the robust states of conformation, and that small controls can induce conformation change by exciting resonances in the dynamics of the nearest neighbor coupling.

Further understanding of the conformation change is gained through a novel approximation that reduces the many degree of freedom system to a coarse $1\frac{1}{2}$ degree of freedom system in which the coarse variables retain precisely the interaction that describes the global conformation change. We demonstrate that the coarse model accurately captures statistics of the conformation change and the effect of various perturbations and controls.

Work with Igor Mezic (UCSB) and Jerrold Marsden (Caltech).

Control algorithms using online simulation. **Radu Balan** (Universitatea Tehnicã Cluj-Napoca, Romania), Vistrian Maties (Universitatea Tehnicã Cluj-Napoca, Romania), Sergiu-Dan Stan (Universitatea Tehnicã Cluj-Napoca, Romania), Olimpiu Hancu (Universitatea Tehnicã Cluj-Napoca, Romania) GA/CT2177/013

Today, many industrial systems are still controlled by simple PID (proportional-integrative-derivative) algorithms, despite the better performances usually provided by systems developed following the modern control theory. This is probably not only due to the quite surprising efficacy of this simple control method, but also to the higher computational load and design effort required by most of the more sophisticated control techniques. PID controllers can be used to control a wide range of different processes, need only rough process models to be easily tuned and give pretty good set-point tracking performances. On the other hand it is clear that PID performances, although satisfactory, could be improved when dealing with highly nonlinear processes, or processes featuring unmodeled dynamics and external disturbances. The paper presents a control algorithm based on the on-line simulation of the future behavior of the control system, by using a few candidate control sequences. Then, using the rule based control, these simulations are used to obtain the ŚoptimalŠ control signal. The efficiency and applicability of the proposed algorithm are demonstrated through applications.

GA/CTS4871/13: Mechanical systems and stability.

Organiser: Peter Eberhard (Universität Stuttgart, Germany)
Co-organiser: Uwe Helmke (Julius-Maximilians-Universität Würzburg, Germany)

An elastic beam approach to predictive vehicle motion planning with low curvatures. **Karina Hirsch** (Universität Duisburg-Essen, Germany), Thorsten Brandt (Universität Duisburg-Essen, Germany) GA/CT1592/013

Vehicle guidance systems are among the latest automotive developments. Examples are automatic cruise control, lane departure warning and active lane keeping. However, the rapid development of environmental sensor systems such as radar, lidar and video technologies in combination with data fusion of the single sensor signals enables further applications as for example lane changing assistance, collision avoidance or even autonomous driving. For all of these functions, trajectories have to be planned and, depending on the application, to be communicated to the driver. Recently, methods originally developed in robotics as for example so-called elastic bands are adopted for road vehicle applications. However, vehicle dynamics are in general not considered in these approaches. Though, for road vehicles at high speeds drivability becomes an important issue: if the curvature of the planned trajectory is locally too high for the intended speed, the vehicle will start skidding. For this reason a new motion planning approach is proposed. The vehicle is guided along a virtual elastic beam, which is deflected by virtual potential fields generated by obstacles in the traffic space. In doing so, the elastic beam avoids obstacles and provides collision-free trajectories. In particular, the flexural stiffness of the beam can be chosen with respect to vehicle dynamics.

Integrated measurement system using accelerometers and gyros as peripheral sensors to estimate the motional state of an elastic beam. **Thorsten Örtel** (Universität Stuttgart, Germany), Jörg Wagner (Universität Stuttgart, Germany) GA/CT1746/013

Integrated navigation devices for vehicle guidance are the most common example of an integrated motional measurement system combining the signals from an inertial measurement unit (three accelerometers, three gyros) and a GPS receiver with a single antenna. Traditionally, the vehicle is assumed to be a single rigid body with six motional degrees of freedom to be determined. During periods of low vehicle dynamics the common integrated navigation systems show stability problems. Nevertheless, the stability of the system can be guaranteed by distributing sensors over the vehicle structure. However, in this case the rigid body assumption has to be expanded to take the distributed sensors and the flexibility of the structure into account.

Integrated systems in general are fusing different measuring signals by combining their benefits and blinding out their disadvantages. For instance, gyros and accelerometers are used to obtain reliable signals with a good time resolution. On the other hand, aiding sensors like radar units and strain gauges are known to be long-term accurate. Furthermore, the kernel of the integrated systems consists of an extended Kalman filter that estimates the motion state of the structure. Besides the sensor signals, the basis for the filter is an additional kinematical model of the structure which has to be developed individually.

The example of the motion of an elastic beam being considered here is meant to be an approach to obtain motional measurements of a wing of a large airplane during flight. By means of a modal approach, a kinematical model of the beam was developed. This paper will compare integrated systems utilising accelerometers as peripheral sensors with systems using gyros and systems with a combination of both peripheral sensor types. Based on simulation the paper shows this approach, different sensor configurations, and estimated motion results of an elastic beam.

Multimodel control approuch for electrohydraulic servo systems. **Olimpiu Hancu** (Universitatea Tehnicã Cluj-Napoca, Romania), Vistrian Maties (Universitatea Tehnicã Cluj-Napoca, Romania), Radu Balan (Universitatea Tehnicã Cluj-Napoca, Romania) GA/CT2760/013

The paper proposes a control design approach based on a multipoint linearization method for linear electro-hydraulic servo systems. The nonlinear model of servo system is linearised around of operational points and Matlab environment is used to adjust the points distribution based on error estimation. These models are used to design an optimal controller which online modifies the feedback control parameters. Simulation and experimental results are provided to show the effectiveness of approach.

Control and stability analysis of a turbocharged diesel engine using singular-perturbation methods. **Hannes Seyrkammer** (Universität Linz, Austria), Kurt Schlacher (Universität Linz, Austria) GA/CT2390/013

This contribution is concerned with the application of a nonlinear control and stability analysis for diesel engines equipped with a variable geometry turbocharger (VGT) and an exhaust gas recirculation (EGR) valve, using singular perturbation methods. The recirculation of exhaust gas from the outtake manifold to the intake manifold is an effective way to reduce the concentration of nitrogen oxides in the exhaust gas. Using a VGT, a fast transient response time at low engine speeds and high engine power without turbine overspeeding at high engine speeds is possible. The system to be controlled is described by the following simple scheme: air enters the system through the compressor and is led to the intake manifold. Mixed with the recirculated gas it is pumped into the engine. Inside, fuel is injected and the combustion takes place. The produced exhaust gas flows into the exhaust manifold. A part is recirculated to the intake manifold, the rest flows through the turbine, transferring energy to the compressor. For the controller design a simplified mathematical representation is given by a set of three ordinary differential equations. These equations can be split into two parts with slow and fast transient response. The goal of the controller is to achieve desired values of the input manifold pressure and the compressor massflow, both given by the motor management system for a given point of operation. To guarantee that the deflection of the desired and actual signals converge to zero, the controller is equipped with two slow integral states. The equations for the closed loop system can be written as a nonlinear standard singular perturbated system. The asymptotic stability is shown with the choice of Lyapunov functions for the reduced and the boundary layer system such that the necessary interconnection conditions are also satisfied. The performance of the controller is demonstrated by simulation results also in combination with a more detailed simulation model.

Controlled piezoelectric actuators in machine tools. **Christian Rudolf** (Universität Karlsruhe (TH), Germany), J Wauer (Universität Karlsruhe (TH), Germany) GA/CT1467/013

In machine tools of parallel structure with two or three translatory degrees of freedom rotatory degrees of freedom are kinematically locked. However, due to geometric faults, such as installation errors or different geometries due to production tolerances, those machine tools suddenly exhibit a full three dimensional behavior resulting in stresses within the structure and leading to deflections of the tool center point. Thus, the quality of the workpiece is reduced.
To compensate these errors an adaptronic strut which can be implemented within such a machine tool has been developed. The strut comprises a piezoelectric sensor-actuator unit for the force controlled correction of those static and quasistatic deflections since piezoelectric elements are advantageous due to their high accuracy and the small installation space required.
Here, a control design for the compensation is presented. After considering a single adaptronic strut as a standalone system with external loads representing constraint forces, the strut is implemented within the machine tool. Then, the effect of the controlled strut on the operating behavior of the machine tool is investigated.

Inversion-based trajectory planning for the heat equation with temperature-dependent parameters and radiation boundary conditions. **Tilman Utz** (Universität des Saarlandes, Germany), Thomas Meurer (Universität des Saarlandes, Germany), Daniel Wild (Universität des Saarlandes, Germany), Andreas Kugi (TU Wien, Austria) GA/CT3453/013

In hot-rolling mills, metal slabs are heated in pusher-type reheating furnaces from the ambient temperature to a final temperature required for the hot-rolling process; see e.g., [1,2]. To meet the metallurgical demands, it is required to reach certain temperature profiles within the slabs along pre-planned temporal paths within a given time interval. Thereby, radiation represents the primary mode of heat transfer within the furnace such that energy is exchanged between the furnace and the slab along the slab surface.

Modelling of the temperature distribution within a slab leads to a description in terms of the heat equation with temperature-dependent heat capacity, mass density and thermal conductivity. Furthermore, in good accordance with physical evidence, it suffices to consider only heat conduction in the vertical direction (i.e., over the height of the slab), which renders the model spatially 1-dimensional[2].

For the solution of the trajectory planning problem, in this contribution an inversion-based approach is applied, which is based on the appropriate semi-discretization of the governing nonlinear heat equation with radiation boundary conditions using Finite Differences with respect to the spatial coordinate. For this, it is assumed that the furnace temperatures above and below the slab can be utilized as the control inputs. Based on the semi-discrete approximation, it is shown that the temperature and its gradient at the core of the slab represent so-called flat outputs of the system[3]. This allows us to parametrize the temperatures at the discrete locations as well as the boundary inputs in terms of the flat outputs and their time-derivatives. Hence, prescribing appropriate trajectories for the flat outputs directly yields the control inputs which are necessary to track the core temperature and its gradient along the prescribed path in open-loop. Furthermore, the parametrizations of the spatially discrete temperatures can be utilized to ensure that the temperature gradient along the slab height remains in an admissible range in order to fulfill the metallurgical requirements on the heating process.

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[3] Fliess, M.; Lévine J., Martin, P. and Rouchon, P.; Int. J. Control. **61** (1995), pp.1327–1361.

14, Minisymposia

GA/MP395/014: Geometric techniques in control.

Organiser: Kurt Schlacher (Universität Linz, Austria)
Co-organiser: Achim Ilchmann (TU Ilmenau, Germany)

Control of port-Hamiltonian systems by interconnection and energy shaping via generation of Casimir functions. **Alessandro Macchelli** (Università di Bologna, Italy), Arjan van der Schaft (University of Groningen, Institute of Mathamatics, The Netherlands), Claudio Melchiorri (Università di Bologna, Italy) GA/MT4238/014

In this talk, an overview on the control by interconnection and energy shaping via Casimir generation for port Hamiltonian systems is presented. This control methodology has its origins in the Energy-Casimir method according to which stability can be proved by using in Lyapunov analysis next to system Hamiltonian other conserved quantities. In the control by interconnection, the controller structure is chosen in order to properly introduce such conserved quantities (Casimir functions) and shape the energy of the system such that a minimum in the desired equilibrium configuration can be introduced. The basic results on the stabilization of finite dimensional systems are summarized and then generalized in order to deal with the infinite dimensional case.

Modeling, simulation and control of a doubly-fed induction machine. **Carles Batlle Arnau** (Universitat Politècnica de Catalunya, Spain), Enric Fossas Colet (Universitat Politècnica de Catalunya, Spain), Arnau Dòria Cerezo (Universitat Politècnica de Catalunya, Spain) GA/MT4240/014

This presentation deals with a complex multidomain system, including the control objectives specification, modeling, control design, simulation, experimental setup assembling and experimental validation stages. The system under study is an energy storage system whose main components are a flywheel, a doubly-fed induction machine and a back-to-back electronic power converter. Along with the study of this specific system, a review is presented of the major techniques employed, namely port Hamiltonian system theory and interconnection and damping assignment-passivity based control, and some original theoretical improvements of the basic control technique are also obtained.

On geometric dynamics of rigid multi-body systems. **Stefano Stramigioli** (Universiteit Twente, The Netherlands) GA/MT4246/014

Standard methods to model multibody systems are aimed at systems with configuration space isomorphic to $\mathfrak{R}^n$. This limitation leads to singularities and other artifacts in case the configuration space has a different topology, for example in the case of ball joints or a free-floating mechanism. The presentation discusses an extension to classical methods to allow for a very general class of joints, that includes all with a Lie group structure, as well as nonholonomic joints. The model equations are derived using the Boltzmann-Hamel equations and have the same structure and complexity as in the standard results, but do not suffer from singularities. Furthermore, they avoid implicit formulations (both for holonomic and nonholonomic joints) and can be directly implemented in simulation software.

On the interconnection structures of discretized port-Hamiltonian systems. **Bernhard Maschke** (Université Claude Bernard Lyon I, France) GA/MT4345/014

Port Hamiltonian systems are an extension of infinite-dimensional Hamiltonian systems which allow to model open physical systems having some exchange of energy with their environment through the boundary of their spatial domain . They are defined on a Dirac structure, called Stokes-Dirac structure, which is an extension of the Poisson bracket associated with the differential operator arising in systems of conservation laws .It has been shown that such Stokes-Dirac structures not only arise in models of conservative systems (in the sense of Thermodynamics) such as vibrating strings or isentropic flows, but also in models of irreversible systems such as diffusion processes or heat conduction . For the purpose of numerical simulation or control, a mixed-finite element method has been developed that preserves the port-Hamiltonian structure of the system . However this method has been applied for systems defined on 1-dimensional spatial domain. In this paper we shall suggest some generalization of these result to higher-dimensional spatial domains by the use of Whitney forms defined on a primary mesh and its dual mesh.

GA/MP395/014: Geometric techniques in control. #2

Organiser: Kurt Schlacher (Universität Linz, Austria)
Co-organiser: Achim Ilchmann (TU Ilmenau, Germany)

(For abstract, see session #1 above.)

Controllability of the double-bracket flow. **Uwe Helmke** (Julius-Maximilians-Universität Würzburg, Germany), Gunther Dirr (Julius-Maximilians-Universität Würzburg, Germany) GA/MT4943/014

We investigate the controllability properties of Brockett's isospectral double bracket flow on selfadjoint projection operators. Generic conditions for accessibility of the flow are proven, using results on the classification of transitive Lie group actions on Grassmann and Lagrange-Grassmann manifolds. Our results imply corresponding accessibility results for the dynamic matrix Riccati equation with multiplicative controls.

Time-variant Hamiltonian control systems: a covariant approach. **Markus Schöberl** (Universität Linz, Austria) GA/MT4952/014

In this contribution we present an intrinsic description of time variant Hamiltonian control systems. This formulation is based on the splitting of the state bundle and the use of appropriate covariant derivatives, which guarantees that the structure of the equations is invariant with respect to time variant coordinate transformations. The analysis of the change of the Hamiltonian along solutions of the system leads to some new perspectives in the time variant setting, which can be analyzed using geometric methods. This is important from the control theoretic point of view, since this is linked closely to the stability analysis. The trajectory tracking problem for time invariant Hamiltonian control systems can be formulated using the developed theory, since the use of displacement or error coordinates fits perfectly into this covariant setting. Furthermore, if the nontrivial state bundle connection can be absorbed in a modified Hamiltonian, the control task to stabilize the tracking error can be handled by standard methods.

Observability of polynomial and analytic nonlinear systems. **Bernd Tibken** (Bergische Universität Wuppertal, Germany) GA/MT5032/014

In recent years the derivation of effective and computationally verifiable criteria for observability of nonlinear systems has gained some interest. In this contribution the observability is defined in a global way using differential geometric conditions it is shown how the well known local results can be derived and the limitations of this approach are clarified. By specializing to polynomial systems some recent results from real algebraic geometry will be applied in order to derive global conditions for observability. It is shown with several examples that these conditions can be tested effectively. The extension of this approach to the important subclass of Pfaffian analytic systems is presented and illustrated with examples. The main tools which are used are differential geometry and algebraic geometry and especially classical ideal theory. The presentation ends with conclusions and an outlook.

14, Short Communications

GA/CTS4816/14: **Thermo-electric and magnetic flow control.**

Organiser: Gunter Gerbeth (Forschungszentrum Dresden–Rossendorf, Germany)
Co-organiser: Michael Hinze (Universität Hamburg, Germany)

Solidifying-crystal solute flow control through thermo-electric–magnetic interaction. **Koulis Pericleous** (University of Greenwich, UK), Georgi Djambazov (University of Greenwich, UK), Andrew Kao (University of Greenwich, UK), Vaughan Voller (University of Minnesota, USA) GA/CT2039/014

Often metals and alloys solidify in the presence of electromagnetic fields that have marked effects on microstructure and finally properties. The process that creates these microstructures is not well understood and therefore possible benefits gained by a deliberate control of the interaction are not realized. This driver motivates this study, where the solutal flow surrounding a growing dendritic crystal is manipulated through the action of an external magnetic field. The magnetic field interacts with the thermoelectric Seebeck currents present along the solid/liquid interface to generate an electromagnetic Lorentz force. This in turn creates a micro-convection field that can alter the morphology and growth rate of the dendrite. The thermoelectric currents are naturally present along the interface, due to temperature differences between the tip and the root of each dendrite branch where solid and liquid Seebeck strengths differ. To simulate this effect, equiaxed dendrites are grown from grains in a supercooled alloy melt, using an enthalpy front-tracking approach due to Voller. VollerŠs microstructure code is embedded into the Finite Volume CFD package PHYSICA, where in addition to enthalpy, equations are solved for velocity and electromagnetic field. The resulting micro-convection has a marked effect on single and multiple dendrite growth patterns.

Thermo-electric currents in weld pools. **Adrian Lange** (Frauenhofer Institut IWS, Germany), Eckhard Beyer (Frauenhofer Institut IWS, Germany) GA/CT3105/014

In order to achieve higher welding speeds and a better quality of the weld seam, external static magnetic fields are tested for laser beam welding. Experiments with fine grained steels and aluminium alloys show a reduction of so called humping effect, an improvement of the top seam quality, and an influence on the cross section of the seam [1,2]. These phenomena depend on the orientation of the magnetic field. To explain that dependence, the existence of thermoelectrical currents was proposed in [1,2]. The interaction of that proposed currents with the external field shall generate a Lorentz force distribution in the weld pool which may be the reason for the observed phenomena.

Based on the Onsager relation for the thermoelectrical current density and the appropriate boundary conditions in the case of laser beam welding, thermoelectrical currents can be determined analytically [3]. Results for iron and aluminium are presented in a approximative two-dimensional geometry. For iron the assumed current density distribution was confirmed qualitatively. For aluminium the calculated strength of the current is in agreement with the experimental measurements. Since measurements for the values of the thermoelectrical (Seebeck) coefficient of both materials are spare, different hypothetical material sets are tested and discussed.

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[3] J. Paulini, G. Simon, and I. Decker, J. Phys. D **23**, 486 (1990).

Subcritical instability of liquid metal channel flow in the presence of a spanwise magnetic field. **Thomas Boeck** (TU Ilmenau, Germany), Dmitry Krasnov (TU Ilmenau, Germany), Maurice Rossi (Université Pierre et Marie Curie, France), Oleg Zikanov (University of Michigan, Dearborn, USA) GA/CT2318/014

The stabilizing effect of a homogeneous magnetic field on the subcritial instability and transition to turbulence in plane Poiseuille flow of an electrically conducting fluid is studied using hydrodynamic stability theory and direct numerical simulations. The magnetic field is oriented in the spanwise direction.

The transition to turbulence depends on the transient growth of non-modal linear perturbations, which are characterized by their stream- and spanwise wavenumbers. The kinetic energy of the velocity perturbations is used to quantify the energy amplification.

In the non-magnetic case, the most amplified perturbations are purely streamwise rolls. As the Lorentz force tends to suppress motion in the spanwise direction, the most amplified perturbations change from streamwise rolls to oblique rolls as the magnetic field increases. For sufficiently strong fields, motion in the spanwise direction is strongly damped and only the two-dimensional Tollmien-Schlichting waves aligned with the magnetic field provide significant transient amplification. The consequences of this damping effect on the transition to turbulence are studied through direct simulations.

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Electromagnetic flow control of glass melts: theoretical contribution. **Cornelia Giessler** (TU Ilmenau, Germany), Andre Thess (TU Ilmenau, Germany) GA/CT1820/014

The goal of our investigations is to show the possibility to control efficiently glass melt flow with Lorentz forces. We report an analytical model to study the main features of the flow and results of coupled 3D-numerical simulations. The flow control with Lorentz forces is a new way to control the flow rate and temperature in forehearth and feeder systems and increase homogenisation in crucibles and melters without contact.
The analytical model mainly consists of the energy equation and the Stokes equation including buoyancy, friction and Lorentz force. The characteristic features of glass melt such as high viscosity and the strong non-linear temperature dependence of the electrical conductivity and viscosity are taken into account. To drive the glass melt with Lorentz forces we impose crossed external current density and external magnetic field density. Altogether we obtain a complicated interplay between the variation of the material parameter, the heat equation and the Stokes equation. One of the most interesting and intriguing effects is bifurcation in the flow characteristics once the Lorentz force and the change of material parameters go through a certain critical value.
The 3D numerical model describes a crucible containing glass melt and two electrodes being inserted into the melt. Thermal convection develops as result of the density differences. With an additional external magnetic field Lorentz force is generated between the electrodes. We show parameter studies for the power input, magnetic field density and the two possible orientations of the Lorentz force. Furthermore, we compare calculations with constant and temperature-dependent electrical conductivity and reveal the importance of correct implementation of this material parameter.
Overall, the model shows that it is possible to control the glass melt flow using externally applied electromagnetic forces efficiently. The results obtained are compared with experimental results [1].

Asymptotic methods for spherically-symmetric MHD α^2-dynamos. **Uwe Günther** (FZ Dresden–Rossendorf, Germany), Oleg Kirillov (Lomonosov Moscow State University, Russian Federation) GA/CT3043/014

We consider two models of spherically-symmetric MHD α^2-dynamos; one with idealized boundary conditions (BCs); and one with physically realistic BCs. As it has been shown in our previous work, the eigenvalues λ of a model with idealized BCs and constant $\alpha-$profile α_0 are linear functions of α_0 and form a mesh in the $(\alpha_0, \Re\lambda)-$plane. The nodes of the spectral mesh correspond to double-degenerate eigenvalues of algebraic and geometric multiplicity 2 (diabolical points). It was found that perturbations of the constant $\alpha-$profile lead to a resonant unfolding of the diabolical points with selection rules of the resonant unfolding defined by the Fourier coefficients of the perturbations. In the present contribution we present new exact results on the spectrum of the model with physically realistic BCs and constant α. For non-degenerate (simple) eigenvalues perturbation gradients are found at any particular α_0. We present a detailed study of the spectral behavior of the α^2-dynamo operator over a family of homotopic deformations of the BCs between idealized ones and physically realistic ones. Furthermore, we demonstrate that although the spectral singularities are lifted, a memory about their locations remains deeply imprinted in the homotopic family of the spectral deformations due to a hidden underlying invariance.

GA/CTS4818/14: Optimal control and design.

Organiser: Roland Griesse (RICAM Linz, Austria)
Co-organiser: Michael Hinze (Universität Hamburg, Germany)
Co-organiser: Gunter Gerbeth (Forschungszentrum Dresden–Rossendorf, Germany)

Optimal control of radiative transport. **René Pinnau** (TU Kaiserslautern, Germany) GA/CT3663/014

A tracking-type optimal control problem for the radiative transfer equation is studied. Necessary and sufficient optimality conditions are derived. Numerical methods for the model equation and its adjoint are presented. Computational results based on a steepest descent method underline the feasibility of our approach.

Optimal experimental design for flow problems. **Thomas Carraro** (Universität Karlsruhe, Germany) GA/CT2047/014

The theory and practice of optimal design of experiments is well known in several areas of engineering. The scope of this optimization technique is the reduction of the uncertainty in the information obtained by experiments. This is attained by an optimal choice of the experimental conditions. We propose a numerical method for optimal experimental design in the context of flow problems assuming a discretization by means of the finite element method.

Optimisation of an entire design chain in aerodynamics. **Andrea Walther** (TU Dresden, Germany), Nicolas Gauger (HU Berlin & DLR Braunschweig, Germany), Carsten Moldenhauer (TU Dresden, Germany) GA/CT1054/014

For optimising the properties of an air foil, we consider the following design chain consisting of four steps: The computation the geometry of the air foil for a given Hicks-Henne parametrisation, the evaluation of the difference of this air foil with respect to a given static geometry, the corresponding deformation of the given grid around the air foil and the computation of the drag using a special version of the flow solver TAU. To apply a calculus-based optimisation method, one has to differentiate the whole design chain with respect to the given parametrisation. We present and analyse first results for a gradient-based approach. Subsequently, we will discuss alternative methods to handle the substantial start-up calculation that results from the entire design chain. This yields different optimisation approaches aiming at a one-shot method.

Stability control in CFD by shape optimization. **Frank Strauss** (Universität Karlsruhe, Germany) GA/CT2409/014

We focus on problems of optimal control and hydrodynamic stability appearing in computational fluid dynamics. In that context we consider shape optimization problems with adequate objective functions subject to eigenvalue constraints. The eigenvalue state equation is given by the Navier-Stokes eigenvalue problem. Analytical issues focusing on existence results for the optimization problem as well as numerical aspects are addressed. Our study encompasses in particular the development of adequate numerical schemes. The complexity of the underlying problems leads to large highly nonlinear problems which are solved by means of techniques relying on high performance computing. Special attention is paid to the parallelization of the numerical methods developed in that framework. Various examples are presented including the design optimization of a racing yacht for the America's Cup.

On pump modular system for automated adjustment and control for axial piston pumps. **Calin Vaida** (Universitatea Tehnicã Cluj-Napoca, Romania), Liviu Ioan Vaida (Universitatea Tehnicã Cluj-Napoca, Romania), Doina Liana Pisla (Universitatea Tehnicã Cluj-Napoca, Romania), Adrian Pisla (Technical University Cluj-Napoca, Romania), Tiberiu Itul (Technical University Cluj-Napoca, Romania), Lucian Nascutiu (Universitatea Tehnicã Cluj-Napoca, Romania) GA/CT1681/014

Axial piston pumps are the most widely used pumps in hydraulic actuation systems. Their technical characteristics make them the best option for most applications starting from industrial machine tools, up to mobile equipments. Thus, the optimization of their functional parameters and their control within the system is of great importance. The paper presents the working principles of the electro-hydraulic adjustment systems for axial piston pumps with variable displacement. Further on, it is described the construction of a modular measuring and control head (developed entirely by the authors) mounted directly on the pump and ensures the achievement of any type of control: flow, pressure, power or their combinations. The measuring head is mounted on the output port of the pump, thus imposing no constructive modifications on the pump. Finally, the authors will present the testing stand and the experimental results obtained during the functioning of a pump equipped with this system under a flow control regime, pointing out the possibility of automation of complex technological processes, using a process computer or a programmable logic controller.

GA/CTS4814/14: Flow control.

Organiser: Michael Hinze (Universität Hamburg, Germany)
Co-organiser: Gunter Gerbeth (Forschungszentrum Dresden–Rossendorf, Germany)

Mathematical methods in MHD flow control. **Roland Griesse** (RICAM Linz, Austria) GA/CT1697/014

Magnetohydrodynamics, or MHD, deals with the mutual interaction of electrically conducting fluids and magnetic fields. In particular, the magnetic fields interact with the electric currents in the fluid and exert a Lorentz force. This feature renders it so phenomenally attractive for exploitation especially in processes involving liquid metals, and in crystal growth.

The tayloring of currents and magnetic fields offers the possibility to drive the fluid in a desired way, e.g., in order to enhance mixing or to achieve flow damping. These goals can be formulated in terms of objective functions, which lead to optimal control problems. The emphasis in this presentation is on mathematical methods for the numerical solution of incompressible MHD optimal control problems.

Memory-efficient implementation of optimal-control problems for the Navier–Stokes equations. **Julia Sternberg** (Universität Hamburg, Germany), Michael Hinze (Universität Hamburg, Germany) GA/CT1000/014

Derivative-based solution algorithms for optimal control problems of the time dependent Navier-Stokes equations require multiple solutions of backward-in-time adjoint systems. Since these adjoint systems depend on the velocity, and thus on forward information, the storage requirement for such solution algorithms is very large.

We propose stable and memory efficient checkpointing techniques for evaluating gradients and Hessian×increment, and present numerical test which demonstrate that huge memory savings are achieved by our approach while the increase in runtime is moderate.

Finally, we discuss some possible future developments.

Optimal control of the free boundary in a two-phase Stefan problem with flow driven by convection. **Michael Hinze** (Universität Hamburg, Germany), Stefan Ziegenbalg (TU Dresden, Germany) GA/CT1018/014

We present an optimal control approach for the solidification process of a melt in a container. The process is described by a two phase Stefan problem including flow driven by convection and Lorentz forces. The free boundary (interface between the two phases) is modelled as a graph.

We control the evolution of the free boundary using the temperature on the container wall and/or the Lorentz forces. The control goal consists in tracking a prescribed evolution of the free boundary. We achieve this goal by minimizing a appropriate cost functional. The resulting minimization problem is solved numerically by a steepest descent method with step size control, where the gradient of the cost functional is expressed in terms of the adjoint variables.

Optimization of compressors in gas networks. **Michael Herty** (TU Kaiserslautern, Germany) GA/CT1045/014

We are interested in optimization issues arising in the context of gas flow in pipeline networks. Here, the dynamics of the flow inside the gas pipes is described by the isothermal Euler equations, i.e. a nonlinear hyperbolic partial differential equation. In physical networks compressor stations are introduced reduce the pressure loss due to wall friction. We present a model for a compressor and discuss optimization of the compressor load with respect to the dynamics governed by the isothermal Euler equations. We present analytical as well as numerical results.

Economical heat transfer. **Szpakowska Szpakowska** (Koszalin University of Technology, Poland) GA/CT3132/014

Heat transfer occurs in all situations involving objects of different temperatures. This paper is devoted to convective heat transfer and accompanying methods of its intensification. If the process could be intensified without any energy outlays, i.e. without the use of energy-consuming elements (fans, blowers), considerable economic benefits could be achieved. These could be employed not only in the industry but also in ordinary households. Nearly all technologies practically used in metallurgical, power, chemical or food industries require the provision or consumption of considerable quantities of heat.Intensification is effected by increasing airflow speed, usually by means of fans requiring a drive system, which entails considerable energy outlays. A number of design solutions of heat exchangers use the phenomenon of convective heat transfer. Heat exchangers of this type do not incorporate any devices producing fluid motion. In addition to that, they are easy to operate, durable and reliable.

GA/CTS4819/14: Ferro fluids.

Organiser: Stefan Odenbach (TU Dresden, Germany)
Co-organiser: Michael Hinze (Universität Hamburg, Germany)
Co-organiser: Gunter Gerbeth (Forschungszentrum Dresden–Rossendorf, Germany)

Free-surface phenomena and flow in ferrofluids. **Reinhard Richter** (Universität Bayreuth, Germany), Christian Gollwitzer (Universität Bayreuth, Germany), Christopher Groh (Universität Bayreuth, Germany), Holger Knieling (Universität Bayreuth, Germany) GA/CT2770/014

The Rosensweig- or normal field instability [1] is one of the most striking phenomena of ferrofluids. Above a threshold B_c of the vertically oriented magnetic induction B_z the initially flat surface gives way to a stationary pattern of liquid crests. Despite its 'advanced age' of 40 years the nonlinear properties of the instability became only recently gaugeable, thanks to use of radioscopy [2].

We measure the amplitude and shape of the hexagonal pattern versus the magnetic induction and compare the results [4] with analytical [3] and numerical treatments of the instability. Moreover we uncover localized states (*ferrosolitons*) in the bistable regime [5], which are recovered by the finite element method [6]. For higher inductions the hexagons are followed by squares via a *proteretic* transition [7]. By adding a horizontal field component B_x the symmetry of the pattern can be broken [3]. For fixed $B_x > 0$ and increasing B_z liquid ridges appear supercritically [8], which are replaced by stretched hexagons via a subcritical bifurcation at higher inductions. Contrary, fixing B_z and increasing B_x shows for the first time a coexistence of two different hexagonal pattern. The instability is measured as well for inverse ferrofluids. Due to their apparent yield stress [9] an elastic energy contribution becomes important, resulting in a shift of B_c to higher values, which is confirmed by theory [10]. Eventually the static surface structures are moved by means of a rotating magnetic field, a *magnetic pump* [11].

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Maximal growth rate at the Rosensweig instability: theory, experiment, and numerics. **Holger Knieling** (Universität Bayreuth, Germany), Adrian Lange (Frauenhofer Institut IWS, Germany), Gunar Matthies (Ruhr-Universität Bochum, Germany), Ingo Rehberg (Universität Bayreuth, Germany), Reinhard Richter (Universität Bayreuth, Germany) GA/CT3062/014

Instabilities in magnetic fluids (MF) have had a long history with the most eye-catching phenomenon being the normal field or Rosensweig instability [1]. When a critical value B_c of the vertical magnetic induction is surpassed, static liquid peaks arranged in a hexagonal pattern are rising on the free surface of the fluid.

A linear description of the Rosensweig instability is amenable in theory, but restricted to small amplitudes. In experiments they can be observed only for a very short time during the increase of the pattern of ridges, which bifurcate supercritically. Thus a new pulse technique has been developed and applied [2,3].

The ground state of a pattern forming system is subjected to small disturbances in order to study its stability. It is assumed that in the linear state of the pattern forming process the wave number with the largest growth rate will prevail. That growth rate is the last remaining quantity which has not been measured and compared to the theoretical results. This contribution is devoted to fill this gap and presents theoretical, experimental, and numerical results for the maximal growth rate for two different MFs. Primarily results show that the experimental and numerical data agree satisfyingly whereas the theoretical data show a sizeable disagreement. The reasons for the latter will be discussed.

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Structure formation and phase behaviour in ferro-fluid monolayers: theory and computer simulations. **Juan Jose Cerda Pino** (Universität Frankfurt, Germany), Christian Holm (Universität Frankfurt, Germany), Sofia Kantorovich (Urals State University, Russian Federation) GA/CT1998/014

Ferrofluid particles are known to self-assemble into a variety of magnetic equilibrium structures which depend on several factors such as: system geometry, magnetic interactions, particle polidispersity, presence or absence of external fields, etc. The phase behaviour and microstructure of ferrofluid systems in reduced dimensions is not necessarilly equivalent to that of 3D systems. In order to investigate the peculiarities brought by the 2D geometry into the aggregation processes in ferrofluids, a combination of density functional theory, and molecular dynamics (MD) simulations is presented. Long-range dipolar interactions in our monolayer simulations are computed using a recently developed dipolar-P3M-layer correction algorithm. In comparison to the traditional Ewald sum methods, this approach allows to handle larger systems. The mircrostructure formation and the phase behaviour of monodisperse and bidisperse ferrofluid monolayers are studied thoroughly. The effects induced by the presence of external fields applied to the ferrofluid monolayers are also studied in detail. An extensive comparison of the theoretical, and computational results to the experimental results from *in situ* cryogenic tansmission electron microscopy [1] will be also presented.

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Locomotion based on the control of the shape of magnetic fluid surfaces and of magnetizable media. **Klaus Zimmermann** (TU Ilmenau, Germany), Vera Naletova (Moscow State University, Russian Federation), Igor Zeidis (TU Ilmenau, Germany), Vladimir Turkov (Moscow State University, Russian Federation), Valter Böhm (TU Ilmenau, Germany), Emil Kolev (TU Ilmenau, Germany) GA/CT1940/014

The realization of locomotion based on the deformation of a free surface of a magnetic fluid layer in a traveling magnetic field is studied. It is known that the traveling magnetic field can create a flux in the fluid layers. The theory of the flow of layers of magnetizable fluids in a traveling magnetic field is considered. A plane flow of an incompressible viscous magnetic fluid layer on a horizontal surface in a nonuniform magnetic field, a plane two-layers flow of incompressible viscous magnetic fluids between two parallel solid planes in a magnetic field, a flow of an incompressible viscous magnetic fluid layer on a cylinder in a nonuniform magnetic field, and other problems are considered. Experiments for the estimation of the forces arising on a surface of a magnetic fluid under the action of a controlled magnetic field are conducted. It is theoretically and experimentally shown that there is a possibility of creating a travelling wave on the surface of the fluid layer by means of a magnetic field. The deformation and the motion of a body made by a magnetizable polymer in an alternating magnetic

field are experimentally studied. The cylindrical body (worm) which is located in a cylindrical tube is considered. It is found that there is an undulation of the worm in a periodic traveling magnetic field of special structure and the worm moves along the tube. In our experiments the maximal worm velocity is 20cm/s. The calculations of the deformation and the velocity of the worm in an applied magnetic field are done. It is shown that the theoretical results agree with the experiments. Calculation of the worm deformation is done using ANSYS. These effects can be used in designing autonomous mobile robots without a hard cover. Such robots can be employed in clinical practice and biological investigations.

Rheological properties of ferrofluids. **Loredana Mirela Pop** (TU Dresden, Germany), Stefan Odenbach (TU Dresden, Germany) GA/CT2924/010

Due to the possibility to change the physical properties of ferrofluids (i.e., long-term stable colloidal suspensions of nanometer-sized magnetic particles in appropriate carrier liquids) by means of moderate magnetic fields, they can be used to solve a wide variety of technical problems. The usage of magnetically controlled fluids requests not only a good knowledge about the basic properties of ferrofluids but also about their behaviour in the presence of magnetic fields. Thus, effects like, for example, field induced changes of fluids viscosity are subject of actual research activities. Experiments made for different ferrofluids under shear flow have shown that an increase of magnetic field strength yields an increase of the fluids viscosity, the so called magnetoviscous effect, while increasing shear rate leads to a decrease of the viscosity. Combining rheological with SANS investigations, a strong connection between structure formation in ferrofluids under the influence of a magnetic field and their macroscopical behaviour has been established. Based on this knowledge and in order to reach the requirements demanded by applications, new fluids, exhibiting stronger dependence of their properties on magnetic fields, have been developed.

While the previous rheological experiments could been successfully performed using a cone plate rheometer, for the investigation of the highly-concentrated ferrofluid samples new problems arise. Thus, for example, even at very low magnetic field strengths spikes are formed on the free surface of the fluid limiting the range of magnetic field strengths for the investigations. To overcome this problem, a specially designed capillary viscometer has been developed. Additionally, this viscometer allows the variation of the direction of magnetic field relative to the fluid flow. This will enable a comparison of the experimental data to the results of a new macroscopical theory made by M. Liu [Muller et all., 2006 J. Phys. 18].

GA/CTS4820/14: Magnetic fluids.

Organiser: Koulis Pericleous (University of Greenwich, UK)
Co-organiser: Michael Hinze (Universität Hamburg, Germany)
Co-organiser: Gunter Gerbeth (Forschungszentrum Dresden–Rossendorf, Germany)

Rheological investigations of ferrofluids with a shear stress controlled rheometer. **Hamid Shahnazian** (TU Dresden, Germany), Stefan Odenbach (TU Dresden, Germany) GA/CT2997/014

Ferrofluids are superparamagnetic suspensions of nanosized magnetic particles with a mean diameter of about 10 nm in appropriate carrier liquids, like water, oil or organic solvents. The magnetic particles are covered with a polymer shell to keep them stable against sedimentation and to prevent agglomeration. One of the most promising properties of ferrofluids is the possibility to significantly influence their behavior by moderate magnetic fields. This allows to use magnetic forces for the control of properties and flow of these liquids, giving rise to numerous technical and biomedical applications. Recent rheological experiments, performed on ferrofluids, have shown strong change of the viscosity (magnetoviscous effect) and the appearance of viscoelastic effects caused by applied magnetic fields. These effects can be explained with chain and structure formation due to interparticle interaction in the presence of a magnetic field. Additionally, with increase of shear rate structures are broken and the relative change of viscosity decreases. This effect is known as shear thinning. In order to explain the effects different theoretical approaches have been developed, which vary in the basic modelling of the fluid and its behaviour. A point in which the predictions of the models differ is the question of the appearance and field dependence of a yield stress in ferrofluids. For the investigations concerning yield stress a shear stress controlled rheometer for ferrofluids has been designed. The results show a dependence of the yield stress on magnetic field strength for different kind of ferrofluids and magnetorheological fluids. Variation of geometry - cone/plate or plate/plate - and distance of the walls in plate/plate geometry of the shear cell give information on the microscopic size of the structures formed by the magnetic particles and its dependence on field strength as well as interparticle interaction.

Parametric modulation of thermal and thermomagnetic convection in magnetic fluids. **Harald Engler** (TU Dresden, Germany), Stefan Odenbach (TU Dresden, Germany) GA/CT2998/014

Magnetic fluids, also called ferrofluids, are suspensions of magnetic monodomain particles with an average diameter of 10 nm in an appropriate carrier liquid such as oil, water or others. The possibility to control the properties of ferrofluids by means of a magnetic field opens an interesting research field in fluid mechanics as well as technical applications in industry.
This work considers heat and mass transfer phenomena especially convection phenomena in a horizontal fluid layer in ferrofluids in the presence of an external time modulated magnetic field. The driving force in thermal convection depends on the temperature difference and geometric boundary. Furthermore, for such a thermal convection system exists a critical temperature difference for which the transfer of heat changes from diffusion to convective flow. In general the driving force in such a convection experiment is constant in time. In the frame of this work the behaviour of the critical temperature in a convection system with periodically modulated driving force has been investigated. Former theoretical investigations predict that the critical temperature of thermal convection depends on the frequency of the driving force. However the experimental realisation of a situation where thermal convection is subjected to a time variable driving force fails due to immense technical problems. For the investigations of the behaviour of the critical temperature the circumstance is used that the driving force in ferrofluids depends on the temperature difference, geometric boundary and additionally on magnetic body forces. This kind of convection is called thermomagnetic convection. The magnetic force in ferrofluids can thus be modulated in time by a modulation of magnetoic field strength leading to the required time dependent driving force. The experimental setup designed for the investigation of thermomagnetic convection under time varying magnetic driving forces as well as first results on the shift of the stability of the system will be presented.

Numerical study of liquid-metal flow in a rectangular duct under the influence of a heterogenous magnetic field. **Egbert Zienicke** (TU Ilmenau, Germany), Evgeny Votyakov (TU Ilmenau, Germany) GA/CT2897/014

We simulated numerically the laminar flow in the geometry and the magnetic field of the experimental channel used by O. Andreev, Y. Kolesnikov, A. Thess, Phys. Fluids **18**, 065108 (2006). This provides detailed information about the electric potential distribution for the laminar regime (numerical simulation) and in the turbulent regime as well (experiment). As follows from comparison of simulated and experimental results, the flow under the magnet is determined by the interaction parameter $N = Ha^2/Re$ representing the ratio between magnetic force, determined by the Hartmann number Ha, and inertial force, determined by the Reynolds number Re. We compared two variants: (i) (Re, N)=(2000,18.6) (experiment), (400,20.25) (simulation), and (ii) (Re, N) =(4000,9.3) (experiment), (400,9) (simulation) and found an excellent agreement for the numerical and experimental distributions of the electric potential. This is true despite of the fact that the experimental inflow is turbulent while that in the simulation is laminar. As a special feature of the electric potential distribution local extrema under the magnets are observed, as well experimentally as numerically. They are shown to vanish, if the interaction parameter falls below a critical value. Another interesting new detail found in our numerical calculations is the appearance of helical paths of the electric current. Using a simplified magnetic field without span-wise dependence, we show that important physical features of the considered problem are sensitive to small variations in the spatial structure of the magnetic field: the local extrema of the electric potential and also the helical current paths dissappear when the simplified magnetic field is used. The structure of the three dimensional velocity field is also investigated, in particular, a swirling flow is found in the corners of the duct caused by Hartmann layer destruction behind the magnets.

Experiment on MHD turbulence at low magnetic Reynolds number. **Rico Klein** (TU Ilmenau, Germany), Alban Pothérat (TU Ilmenau, Germany) GA/CT2952/014

The work presents an experimental set-up of a scientific experiment concerning the 2D /3D MHD-turbulence transition mechanism in a cubic box, filled with the liquid metal alloy GaInSn and under an imposed constant magnetic field. We discuss the basic construction of our turbulence-box as well as we present first measurement results concerning the 2D/3D transition in MHD turbulence.Basically our box is designed as a modular system, consisting of a polyamid coated cubic brazen frame (inner side length 100mm, electrically insulated) with the respective side plates. On the particular sides of the cubic frame, perpendicular to the magnetic field direction, we install also varnish coated Copper-plates with integrated cards. These cards contain the flow generating mechanism by means of a constant electric current forcing over 100 uniform arranged Copper-electrodes, as well as the high number of 392 electric potential probes, connected to a single ended amplifier system.By real time measurements of the electric potential distribution on both Ha-walls, everyone with the same arrangement and number of 196 electric potential probes, we are able to determine the velocity profile and their high frequency fluctuations as well as we can check the 2D/3D transition, depending on the amount of the injected constant electric current and the magnetic field strength. To check the principal functionality of the experimental set-up and especially the precision of our signal processing system we perform an experiment in smaller scales. The small scale experiment consists of a closed cylindrical box (diameter d= 40 mm), filled with the liquid metall GaInSn (hight h = 5 mm), imposed under a strong magnetic field. The flow is generated by constant electric current forcing over two electrodes and the velocity profiles are measured by 56 electric potential probes on both Ha-walls.We present first results concerning the measurement precision(1 microVolt)and some characteristics of the flow.

GA/CTS4815/14: Flow and magnetic fields.

Organiser: Andre Thess (TU Ilmenau, Germany)
Co-organiser: Michael Hinze (Universität Hamburg, Germany)
Co-organiser: Gunter Gerbeth (Forschungszentrum Dresden–Rossendorf, Germany)

Electromagnetic flow control in weakly conducting fluids. **Tom Weier** (Forschungszentrum Dresden–Rossendorf, Germany), Christian Cierpka (Forschungszentrum Dresden–Rossendorf, Germany), Victor Shatrov (Forschungszentrum Dresden–Rossendorf, Germany), Gerd Mutschke (Forschungszentrum Dresden–Rossendorf, Germany), Gunter Gerbeth (Forschungszentrum Dresden–Rossendorf, Germany) GA/CT1719/014

Electromagnetic (i.e., Lorentz) forces can be used to control the flow of conducting fluids. This holds true even if the electrical conductivity is only weak, as in the case of electrolytes like sea-water.

The applications of streamwise, wall parallel Lorentz forces to generic flow configurations will be exemplified with experimental data from flat plate boundary layers and separated flows around cylinders and hydrofoils. These results demonstrate the ability of stationary Lorentz forces to change the velocity profile in boundary layers and thereby to improve their stability properties, as well as to completely suppress separation. Time dependent Lorentz forces are used to mitigate the lift loss and drag increase of hydrofoils caused by flow separation. In this case, the versatility of Lorentz force actuators allows for detailed experimental investigations especially of the effects of excitation frequency and wave form.

Finally, the impact of the low conductivity on the energy balance of Lorentz force actuators is discussed.

Control of a boundary layer separation. **Vaclav Uruba** (Czech Academy of Sciences, Czech Republic), Lukas Popelka (Czech Academy of Sciences, Czech Republic), Martin Knob (Czech Academy of Sciences, Czech Republic) GA/CT1921/014

Process of a flat-plate boundary layer separation is controlled using a synthetic jet. The boundary layer is subjected to adverse pressure gradient. Synthetic jet is located in the wall, oriented perpendicularly to the flow, the piezoceramic actuator is used. Dynamics of the separation process as well as the synthetic jet / cross flow interaction is studied experimentally using Time Resolved PIV technique.

Experimental results on unsteady boundary layer separation and control mechanism are to be presented. The proper orthogonal decomposition (POD) and bi-orthogonal decomposition (BOD) techniques are involved to study both topological and temporal aspects of the phenomenon. Influence of excitation parameters, namely the synthetic jet position, frequency and its intensity, on control process is to be studied qualitatively as well.

The experimental results will serve as a database to built a simplified mathematical model of the phenomenon.

Numerical simulations of a cylinder wake under a strong axial magnetic field . **Vincent Dousset** (TU Ilmenau, Germany), Alban Pothérat (TU Ilmenau, Germany) GA/CT2962/014

The study deals with the flow past a circular cylinder in a high magnetic field. The magnetic field is imposed along the cylinder axis. The quasi-2D flow model from Sommeria and Moreau (1982) is used. Finite-volume based computations are achieved to simulate the flow for six values of the magnetic field ($0 < B < 1.35T$) and $\mathrm{Re} < 6000$. In the MHD simulations, four successive flow regimes are found. The introduction of the magnetic field delays the apparition of the flow regimes. Few differences are noticed between the hydrodynamic case and the MHD cases concerning the steady flow regime. Concerning the MHD cases, scaling laws in $\mathrm{Re}/\mathrm{Ha}^{\alpha}$ were systematically found in terms of base pressure and drag coefficients, Strouhal number and length of the recirculation regions. Finally, the size of the boundary layer which surrounds the recirculation regions in the steady flow regime is proved to be of the order of magnitude of the characteristic length of the parallel layers.

Work done in collaboration with Alban Pothérat from the Technical University of Ilmenau.

On magnetohydrodynamic drag reduction and flow control behind a body. **Gunter Gerbeth** (Forschungszentrum Dresden–Rossendorf, Germany), Victor Shatrov (Forschungszentrum Dresden–Rossendorf, Germany) GA/CT2167/014

In the first part we present results of direct numerical simulations on turbulent channel flow drag reduction using electromagnetic forces. The Lorentz force is created by the interaction of a permanent magnetic field and an electric current from electrodes placed on the bottom wall surface. We consider the two cases of a spanwise oscillating force and a streamwise steady force. In the second part the flow behind an electromagnetically self-moved sphere is considered for which a drag reduction is found. Results on the linear and nonlinear flow stability will be provided.

Structure of the wake of a magnetic obstacle. **Evgeny Votyakov** (TU Ilmenau, Germany), Egbert Zienicke (TU Ilmenau, Germany), Andre Thess (TU Ilmenau, Germany) GA/CT1842/014

We describe vortices appearing in a liquid metal which flows through and around a magnetic obstacle; i.e., a region where an inhomogeneous magnetic field is applied. This region is featured by the braking Lorentz force due to an interaction of the electrically conducting flow and external magnetic field. Depending on the relationship between viscous, Lorentz and inertial forces, the liquid metal flow shows three different regimes: (1) no vortices, when viscous force prevails at small Lorentz force, (2) one pair of *magnetohydrodynamic* vortices between the magnetic poles, when Lorentz force is high and inertia small, and (3) three pairs, namely, magnetohydrodynamic as above, *connecting*, and *attached* vortices, when Lorentz and inertial forces are high. The attached vortices are similar those which are in usual hydrodynamics in the stagnant region of the flow past a solid cylinder. Since the magnetohydrodynamic and attached vortices are co-rotated, such a motion requires contrrotation between them and this originates connecting vortices. When the inertia force is even higher than in the case (3), then attached vortices develop a vortex breakdown. All types of vortices are found in 3D numerical simulation and confirmed by a physical experiment. Global stability diagrams are discussed.

GA/CTS4817/14: Electro-magnetic flow.

Organiser: Tom Weier (Forschungszentrum Dresden–Rossendorf, Germany)
Co-organiser: Michael Hinze (Universität Hamburg, Germany)
Co-organiser: Gunter Gerbeth (Forschungszentrum Dresden–Rossendorf, Germany)

Electromagnetic flow measurement. **Andre Thess** (TU Ilmenau, Germany) GA/CT1702/014

Electromagnetic fields can be used in a variety of ways to measure the velocity of electrically conducting fluids. Whereas inductive flowmeters provide a convenient and commercially successful means to measure velocities in low temperature fluids like beverages, chemicals, and wastewater, flow measurement in high temperature melts has remained a largely unsurmounted challenge up to now. The present communication will discuss various non-contact methods for flow measurements at high temperature. It will particularly focus on a method, called Lorentz force velocimetry, which consists in measuring the force on a magnet system that interacts with a flow. The advantages and drawbacks of the method will be discussed and an outline of potential applications will be given.

2D and 3D transition of forced MHD turbulence. **Vitali Dymkou** (TU Ilmenau, Germany), Alban Pothérat (TU Ilmenau, Germany) GA/CT3041/014

We consider the incompressible Navier–Stokes equations under an externally imposed magnetic field. The Navier-Stokes equations are taken on the 3D periodic box. The aim is to show the mechanisms which govern the transition between two-dimensional (2D) and three-dimensional (3D) turbulence. We present numerical simulation results using standard pseudo-spectral methods.

Free-surface instabilities during electromagnetic shaping of liquid metals. **Christian Karcher** (TU Ilmenau, Germany), Vaclav Kocourek (TU Ilmenau, Germany) GA/CT2179/014

Electromagnetic shaping of free surfaces of liquid metals is a well-known EPM technology used in a couple of metallurgic processes like cold crucible melting, semi-levitation, and electromagnetic slit sealing, among others. However, the stability of such free surfaces is the most important problem and stability control is crucial for success. Within this context we investigate experimentally the stability behavior of liquid metal free surfaces submitted to a high-frequency magnetic field. The magnetic field is generated by a ring-like inductor fed by an alternating electrical current of high frequency of up to 300 kHz. In this case, the induced Lorentz forces act as an electromagnetic pressure directly on the free surface of the liquid metal. We consider two experimental model configurations: (i) Liquid metal drops placed on a non-conducting plate and (ii) liquid metal discs placed between two horizontal non-conducting plates. As a test liquid we use Galinstan which is liquid at room temperate. The surface contours are observed using a high-speed camera system. The data are analyzed by utilizing both image and signal processing methods. In the experiments we control both electromagnetic parameters, i.e. the inductor current I and the current frequency f, as well as geometric parameters, i.e. drop volume V and disc height H, respectively). In the model configuration (i), upon increasing the inductor current we first observe a static drop squeezing. However, when the inductor current exceeds a certain critical value, these symmetric states become unstable to azimuthal waves. The amplitude, mode number, and oscillation frequency of the observed waves depend strongly on the control parameters. In the model configuration (ii) we observe only static large-amplitude deformations. Upon increasing the current, the ini-

tially circular disc undergoes a series of instabilities as it is deformed in a keyhole-type shape (mode 1), a boomerang-type shape (mode 2), a cloverleaf-type shape (mode 3), and a x-type shape (mode 4). These regular shapes are followed by several irregular shapes of even higher mode number including disc rupture.

Quasi-2D perturbations in duct flows under transverse magnetic field. **Alban Pothérat** (TU Ilmenau, Germany) GA/CT3068/014

Inspired by the experiment from iMoresco and Alboussiere (2004), we study the stability of a flow of liquid metal in a rectangular, electrically insulating duct with a steady homogeneous magnetic field perpendicular to two of the walls. In this configuration, the Lorentz force tends to eliminate the velocity variations in the direction of the magnetic field. This leads to a quasi-two dimensional base flow with Hartmann boundary layers near the walls perpendicular to the magnetic field, and so-called Shercliff layers in the vicinity of the walls parallel to the field. Also, the Lorentz force strongly opposes the growth of perturbations with a dependence along the magnetic field direction. On these grounds, we represent the flow using the model from Sommeria and Moreau (1982), which essentially consists of two-dimensional motion equations with a linear friction term accounting for the effect of the Hartmann layer.

The simplicity of this quasi-2D model makes it possible to study the stability and transient growth of quasi-two dimensional perturbations over an extensive range of non-dimensional parameters and reach the limit of High magnetic fields. In this asymptotic case, the Reynolds number based on the Shercliff layer $\mathrm{Re}/H^{1/2}$ becomes the only relevant parameter. Tollmien–Schlichting waves are the most linearly unstable mode as for the Poiseuille flow, but for $H \gtrsim 42$, a second unstable mode, symmetric about the duct axis, appears with a lower growth rate. We find that these layers are linearly unstable for $\mathrm{Re}/H^{1/2} \gtrsim \mathrm{Re}_c/H^{1/2} = 48350$ and energetically stable for $\mathrm{Re}/H^{1/2} \lesssim 65.32$. Between these two bounds, some non-modal quasi-two dimensional perturbations undergo some significant transient growth (between 2 and 7 times more than in the case of a purely 2D Poiseuille flow, and for much more subcritical valuesof Re). In the limit of a high magnetic field, the maximum gain $G_{\max}$ associated to this transient growth is found to vary as $G_{\max} \sim (\mathrm{Re}/\mathrm{Re}_c)^{2/3}$ and occur at time $t_{G\max} \sim (\mathrm{Re}/\mathrm{Re}_c)^{1/3}$ for streamwise wavenumbers of the same order of magnitude as the critical wavenumber for the linear stability.

Laminar–turbulent transition control of unsteady boundary layer on porous surface in a high fluid-flow acceleration. **Decan Ivanovic** (University of Montenegro, Montenegro and Serbia) GA/CT3296/010

The behavior of a boundary layer in the presence of a positive or negative pressure gradient along the surface is particularly important for the calculation of the surfaces drag as well as for the understanding of the processes which take in a diffuser section, because there is transition from laminar to turbulent flow which determines the dividing line between a region with low drag and one where drag is dramatically increased. So one can control laminar-turbulent transition and shear stress distribution by fluid which has been ejected or injected through the porose surface and this separation reduce is very important goal of flow manipulation. Apart from shear stress we are interested in knowing whether the boundary layer will separate under given circumstances and if so, we shall wish to determine the point of separation. The existence of a negative and in particular of a positive pressure gradient exerts a strong influence on the formation of laminar or turbulent layers. Generalized similarity method is used for calculation of this phenomena. Similar solutions of the boundary layer equations play an important role in the investigation of the stability of hydrodynamic flows and in developing semi-empirical crireria for the transition to turbulence. Through the porose surface in perpedicular direction the fluid of the same properties as incompressible fluid in basic flow, has been injected or ejected with velocity as a function of the contour longitudinal coordinate and time.The corresponding equations of unsteady boundary layer, by introducing the appropriate variable transformations, momentum and energy equations and two similarity parameters sets, being transformed into so-called universal, i.e. generalized for. These parameters are expressing the influence of the outer flow velocity, the injection or ejection velocity, and the flow history in boundary layer, on the boundary characteristics. Solutions, obtained by Tridiagonal Algorithm Method, are used to calculate the characteristic properties: velocity and vorticity distributions, shear stress, momentum and displacement thickness of unsteady boundary layer on porous aerofoil, especially near by separation point. It's found that for both in confuser and in diffuser aerofil regions the accelerating flow increases the shear stress and postpones the boundary layer separation, i.e. laminar-turbulent transition section.When the unsteady parameter is increasing the shear stess magnitude is increasing on whole aerofoil contour and the separation is removing along the surface. It means that the positive local acceleration leads to the postponing of the boundary layer separation in the diffuser region from 70

ICIAM 07 Congress Talks

00 Invited Speakers

01 Computing
(including: computational science and engineering, scientific computing, parallel computing, high performance computing, information technology, software engineering, the Web)

- 010: General
- 011: Knowledge and information systems
- 012: Numerics, algorithms
- 013: Data analysis and visualisation
- 014: Collaboration tools
- 015: None of the above, but in this section

02 Numerical Analysis
(including: numerical linear algebra, numerical methods for ODEs, DAEs, and PDEs, mesh generation)

- 020: Numerical linear algebra
- 021: Numerical methods for interpolation and approximation
- 022: Numerical methods for quadrature
- 023: Numerical methods for integral equations
- 024: Numerical methods for ODEs and DAEs
- 025: Numerical methods for PDEs: evolution problems
- 026: Numerical methods for PDEs: stationary problems
- 027: Mesh generation, adaptive methods, multigrid
- 028: Alternative discretisation methods
- 029: None of the above, but in this section

03 Nonlinear Analysis and Dynamical Systems
(including: bifurcations, nonlinear oscillations, hysteresis, solitons and multivariate solitons, chaos)

- 030: Integrable systems, solitons, control theory
- 031: Statistical methods
- 032: Nonlinear time-series
- 033: Nonlinear PDEs and ODEs, oscillations
- 034: Geometric aspects, symmetries
- 035: Classical and quantum chaos
- 036: Model systems, diffusion, biological systems
- 037: Global structure, hyperbolicity
- 038: Lyapunov stability

039: None of the above, but in this section

04 Partial Differential Equations linear and non-linear

040: Reaction-diffusion equations, steady-state solutions, bifurcation

041: Asymptotic solutions, asymptotic domain decomposition

042: Regularity theory, well-posedness

043: Iterative methods, functional differential equations

044: Blow-up problems

045: Free-boundary problems

046: Conservation laws, symmetries

047: Inverse problems, ill-posed problems

048: Spectral problems, stability, scattering

049: None of the above, but in this section

05 Applied Analysis
(including: integral equations, functional equations, Fourier analysis, wavelets, asymptotics, perturbation methods, special functions, evolution problems)

050: Wave propagation, scattering

051: Coupled systems

052: Asymptotics, perturbation theory

053: Complementarity

054: Wavelets

055: None of the above, but in this section

06 Optimization
(including: control theory, systems theory, operations research, stochastic optimization)

060: General

061: Optimization with PDEs

062: Control and robustness for nonlinear dynamical systems

063: Algorithms and applications of nonlinear optimization

064: Complementarity, equilibrium problems, variational inequalities

065: Ill-conditioned, inverse and saddle-point problems

066: Scheduling, inventory, graphs and discrete optimization

067: Global, multi-objective and robust optimization methods

068: Security and defence

069: None of the above, but in this section

07 Discrete Mathematics
(including: integer programming, networks)

070: General

071: Coding theory

072: Networks, graphs

073: None of the above, but in this section

08 Probability and Statistics
(including: stochastic PDE, telecommunications, financial mathematics)

080: General

081: Statistical Inference

082: Linear models
083: Design of experiments
084: Data analysis, data mining, inverse problems
085: Computational methods
086: Monte Carlo methods
087: Stochastics, processes, analysis
088: Finance
089: None of the above, but in this section

09 Solid Mechanics
(including: material properties, composite materials, soil mechanics, particulate flow, plasticity, structures)

090: Crystals
091: Manufacturing/industry
092: Material interfaces, composites, microstructure, smart materials
093: Granular material
094: Waves, vibrations, cracks, shocks
095: Body dynamics
096: Theoretical topics, special computations
097: None of the above, but in this section

10 Fluid Mechanics
(including: turbulence, aeronautics)

100: Porous media
101: Waves, free surfaces, stratified fluids
102: Stabilitiy theory
103: Incompressible flows and non-Newtonian flows
104: Compressible flows
105: Fluid-strucuture interaction, moving boundary
106: Computational fluid dynamics
107: Convection, heat and mass transfer, mixing
108: Films, jets, surface tension

11 Chemistry and Materials
(including: molecular modelling, polymers, chemical engineering)

110: Ab initio computations
111: Molecular modelling
112: Polymers
113: Chemical engineering
114: None of the above, but in this section

12 Bio-Mathematics
(including: agricultural applications, medical applications)

120: General
121: Ecology, epidemiology
122: Biophysics
123: Tumor and cardiac modelling
124: DNA sequencing, gene technology

125: Other medical applications

126: None of the above, but in this section

13 Physics and Electrical Engineering
(including: electromagnetics, semiconductors, circuit analysis)

130: General

131: Electromagnetics and photonics

132: Semiconductor device simulation

133: Circuit analysis

134: None of the above, but in this section

14 Computational Sciences
(including: meteorology, climate modelling, earthquake, sciences, cosmology)

140: General

141: Meteorology,

142: Climate modelling,

143: Earthquake prediction

144: Tsunami prediction

145: Astrophysics

146: Cosmology

147: None of the above, but in this section

15 Modelling and Simulation for Industry
(including: combustion theory, heat transfer, engineering applications, inverse problems)

150: General

151: Manufacturing

152: Minerals/metals

153: Combustion

154: Microscale, porous media

155: Inverse problems

156: Fluids

157: General

158: Security/defence

159: None of the above, but in this section

16 Pure Mathematics

160: General

161: Abstract Algebra and Number Theory

162: Geometry and Topology

163: Analysis, including real, complex, functional and harmonic analysis

164: Logic and Category Theory

165: None of the above, but in this section

17 Mathematics and Computing Education, Culture and History

170: History of mathematics and computing

171: Mathematics, computer science education

172: Computational science education

173: Recreational mathematics

174: None of the above, but in this section

00: ICIAM Invited Lectures

ICIAM Invited Lectures

IC/IT4980: *Dissipation inequalities in systems theory: past, present and future*
Frank Allgöwer (Universität Stuttgart, Germany)

Dissipation inequalities play a fundamental role in systems and control theory and dissipativity is a very useful concept in the analysis and design of nonlinear control systems. They were introduced in the early 1970s as a generalization of Lyapunov inequalities to systems having inputs and outputs. While Lyapunov functions serve to show the stability of dynamical systems, dissipation inequalities can be applied more widely, depending on the choice of the so-called supply rate. Classical cases being for example the well-known passivity or the L_2-norm characterization of nonlinear systems. Like in Lyapunov theory the biggest problem in applications is the construction of the storage function, which is the generalization of the Lyapunov function. However, for certain system classes, storage functions can be constructed systematically using for example backstepping techniques or recently developed tools from the area of computational semi-algebraic geometry, namely semi-definite programming and the sum of squares decomposition.

In this talk we will give a brief historical perspective and an introduction to the system theoretic concept of dissipation inequalities. We will present some recent results on dissipation inequalities; e.g., minimum phase analysis, stability analysis of nonlinear differential algebraic equation (DAE) systems, and nonlinear feedback and observer design that are based on novel dissipation inequalities and we will discuss questions concerning the computation of the storage functions. The methods will be demonstrated and critically assessed with various examples from engineering and systems biology.

IC/IT4959: *Compressive sampling*
Emmanuel Candès (California Institute of Technology, USA)

One of the central tenets of signal processing and data acquisition is the Shannon–Nyquist sampling theory: the number of samples needed to capture a signal is dictated by its bandwidth. Here we introduce a novel sampling or sensing theory which goes against this conventional wisdom. This theory, now known as *Compressed Sensing* or *Compressive Sampling*, allows the faithful recovery of signals and images from what appear to be highly incomplete sets of data; i.e., from far fewer measurements or data bits than used by traditional methods. We will present the key ideas underlying this new sampling or sensing theory, and will survey some of the most important results. We will emphasize the practicality and the broad applicability of this technique, and discuss what we believe are far reaching implications; e.g., procedures for sensing and compressing data simultaneously and much faster. Finally, there are already many ongoing efforts to build a new generation of sensing devices based on compressed sensing and we will discuss remarkable recent progress in this area.

IC/IT4881: *High-order methods for PDE's: recent advances and new perspectives*
Claudio Canuto (Politecnico di Torino, Italy)

Various paths (such as the hp-version of FEM or the spectral methods) have led over the years to the development of high-order discretization methods for boundary-value problems, which by now can be viewed under a unifying perspective.

We will discuss different issues related to the use of high-order methods. They include the design of efficient elemental bases, particularly in non-tensorial elements; the influence of the local parameters of meshsize and approximation order upon coercivity and $\inf$–$\sup$ constants, as well as *a-priori* and *a-posteriori* error bounds; the adoption of flexible domain partition strategies and the performance of the related algebraic solvers.

We will consider several applications, among which is the discretization of stochastic partial differential equations by means of high-order methods in the stochastic variables.

IC/IT4785: *Greedy algorithms: theory, applications and open problems*
Albert Cohen (Université Paris VI, France)

This talk will discuss computational algorithms that deal with the following general task: given a function f and a dictionary D of functions in a Hilbert space, extract a linear combination of N functions in D which best approximates the function f. In order to avoid combinatorial complexity, these algorithms use a greedy search for selecting the appropriate elements in the dictionary. We shall analyze their convergence properties as N tends to infinity, and discuss applications in various fields such as data compression, statistical learning theory and compressed sensing.

IC/IT4714: *Some fundamental issues in multi-scale modeling*
Weinan E (Princeton University, USA)

I will discuss two representative problems in multiscale modeling: the first is PDEs with multi-scale data; the second is multi-physics modeling. The first problem will be illustrated using standard elliptic equations with multi-scale coefficients. When the participating scales are separated, homogenization theory provides a very effective tool for reducing the complexity of such problems. We will address the question: What can we do when there is no scale separation or any other obvious structure that one can take advantage of in the coefficients? We will discuss a general principle for addressing questions of this

type, and the relevant mathematical and algorithmic issues.

The second problem will be illustrated using continuum and quantum mechanical models of solids such as tight binding models or density functional theory. Questions that will be addressed include: How do we obtain continuum models from quantum mechanical models? How do we formulate coupled quantum/continuum models? How do we design efficient algorithms? The answer to these questions relies on a mathematical understanding of the quantum mechanical models.

IC/IT4501: *Introduction to persistent homology*
Herbert Edelsbrunner (Duke University, USA)

Persistent homology is an algebraic tool for measuring topological features of shapes and functions. It casts the multi-scale organization we observe in nature into a mathematical formalism. This talk will introduce the basic concepts, present a few applications, and survey extensions of the original concept motivated by applications.

IC/IT4967: *New developments in dynamic pricing and hedging and measuring financial risk*
Nicole El Karoui (École Polytechnique, Palaiseau, France)

A large number of strategies are proposed on financial markets to control risks induced by market trend and market fluctuations. Traditional or more sophisticated (exotic) financial products are used by businesses or investors to transfer their risks to financial institutions.

Important questions faced by the market risk industry; e.g., the development of asset pricing models and hedging strategies based on daily (infinitesimal) risk management criteria, have found answers through probabilistic tools and concepts, such as Brownian motion, martingales, and stochastic control and related fields. This in turn has had an important impact on the (exponential) development of this industry.

Numerical implementation is the cornerstone of the modelling process. The choice of a model is hence driven not only by its theoretical properties but also, and in great part, by its numerical tractability. This includes, among other things, reliable estimation of parameters, which are inferred from observable market data (financial products prices). Over the last few years, techniques for stabilizing these ill-posed problems via fast and accurate algorithms in partial differential equations have been developed. In other respects, with motivation coming from multidimensional problems, Monte Carlo methods have been revisited in order to obtain accurate numerical results for prices of high-dimensional products or their derivatives with respect to key parameters. Efficient methods are based on differentiation on Wiener space and Malliavin calculus. A recent topic is that of solving optimization problems (optimal stopping times, optimal portfolio) through Monte Carlo methods.

Thanks in part to the size reached by derivatives markets, market authorities now require financial institutions to compute their daily global exposure (Value at Risk) via their own *internal* models. Motivated by this challenge, academic and risk-managers are debating the *best concept* of risk measure and various problems induced by the high-dimensional character of the covariance matrices they deal with. Mathematical finance is a challenging and fast evolving domain, constantly looking for new ideas and concepts in Mathematics. One of its very remarkable aspects is the ability of theoretical research to have direct implications on daily market practice.

IC/IT4440: *Order-value optimization and new applications*
José Mario Martínez (Universidade Estadual de Campinas, Brazil)

Order-value optimization (OVO) is a family of problems in which the objective function depends of the relative position of a set of real components for each point in the domain. These problems are generally difficult because convexity and smoothness of the components are not inherited by OVO objective functions. Primal methods that converge to suitable defined stationary points have been developed. Reformulations of OVO as smooth (and large) nonlinear programming problems are also available. Applications include robust parameter estimation, risk minimization, protein alignment, structural alignments, computer vision, separate-variable optimization, and many others.

IC/IT4965: *Pattern formation in micromagnetics*
Felix Otto (Universität Bonn, Germany)

Micromagnetics deals with the spatial pattern formed by the magnetization of a ferromagnet. From the point of view of mathematics, micromagnetics is an ideal testbed for a pattern-forming system in materials science: There are abundant experiments on a wealth of visually attractive phenomena and there is a well-accepted continuum model.

In this talk, I will focus on a couple of specific experimental pattern for thin film ferromagnetic elements. Starting point for our investigation is the micromagnetic model which has several characteristic length scales and thus many parameter regimes. For the pattern under consideration, we identify the appropriate paramater regime and rigorously derive a reduced model. We analytically investigate and numerically simulate the reduced model and compare its predictions to experimental data from our collaborators.

IC/IT4788: *Computing, business and applied mathematics: the next challenges*
William Pulleyblank (International Business Machines (IBM), USA)

There have been two consistent drivers over the last sixty years of the evolution of computing: Computer power and price/performance improve by a factor of two every eighteen months; the problems that we wish to solve require this growth in capability and more.

We seem to be reaching inflection points with both of these drivers. High performance systems are resorting to massive parallelism to continue the required growth in performance. The new challenges arising in business and industry are requiring the solution of fundamentally different problems as well as the development of new approaches to old problems.

I will discuss both of these issues and some approaches that are being applied, with varying degrees of success. In particular, I will focus on some of the challenges that arise in telecommunications, particularly related to the business models. I will also discuss what I believe are some of the significant challenges that we will face in the future.

IC/IT4485: *Sampling function space: applications and algorithms*
Andrew Stuart (University of Warwick, UK)

Many problems arising in applications require the sampling of a measure on function space. A particular structure that often arises is when the measure has Radon–Nikodym derivative with respect to a Gaussian measure. We introduce MCMC methods for sampling such measures, and study their complexity as a function of the dimension n of the approximating space. The measures in question may be viewed as having a multiscale structure in which a spectrum of scales is present. This spectrum is manifest in the Kahunen–Loeve representation of the reference Gaussian measure.

We start the talk with various illustrations from the fields of econometrics, transition path sampling, signal processing and data assimilation. We then illustrate the unifying mathematical structure underlying all these problems. This leads naturally into the study of algorithms for such problems, and their computational complexity.

IC/IT4734: *Network formation games*
Éva Tardos (Cornell University, USA)

Large computer networks such as the Internet are built, operated and used by a large number of diverse and competitive entities. In light of these competing forces, it is surprising how efficient these networks are. It is an exciting challenge to understand the success of these networks in game theoretic terms: what principles of interaction lead selfish participants to form such efficient networks? In this talk we present a number of network formation games. We focus on simple games that have been analyzed in terms of the efficiency loss that results from selfishness.

IC/IT4962: *Minimum-volume ellipsoids: applications, duality and algorithms*
Michael Todd (Cornell University, USA)

We consider the problem of finding a minimum volume ellipsoid containing a finite set of points in $\mathbb{R}^d$. This problem has applications in data analysis (clustering, detection of outliers or a small core set), robotics (detecting collisions), and statistics (its dual is the optimal design problem). It has a rich duality theory, which suggests effective algorithms. For large-scale problems, first-order methods exploiting the structure of the problem are most efficient; while these were discovered in the '70s, they were rediscovered recently and their computational complexity and asymptotic convergence analyzed.

IC/IT4947: *How to make invisible objects visible and visible objects invisible*
Gunther Uhlmann (University of Washington, USA)

We will describe the method of complex geometrical optics and its applications to find acoustic, quantum, and electromagnetic parameters of a body by making measurements at the boundary of the body. We will also survey recent results on how to make objects invisible to electromagnetic waves.

IC/IT4506: *Nonlinear problems involving integral operators*
Luis Caffarelli (University of Texas at Austin, USA)

We will present several problems and approaches to treat nonlinear problems involving integral diffusions, more precisely, fractional powers of the Laplacean: regularity and stability of solutions and free boundaries for free-boundary problems coming from boundary control, semi-permeable membranes, and constrained Levi processes.

IC/IT4751: *Parabolic PDEs and deterministic games*
Robert Kohn (Courant Institute, NYU, USA)

We usually think of parabolic partial differential equations and first-order Hamilton–Jacobi equations as being quite different. Parabolic equations are linked to random walks, and often arise as steepest-descents; Hamilton–Jacobi equations have characteristics, and often arise from optimal control problems.

In truth, these equations are not so different. I will discuss recent work with Sylvia Serfaty, which provides deterministic optimal-control interpretations of many parabolic PDE. In some cases, for example motion by curvature, the optimal control viewpoint is very natural, geometric, and easy to understand. In other cases, for example the linear heat equation, it seems a bit less natural, and therefore even more surprising.

IC/IT4755: *Recent trends in robust convex optimization*

Arkadi Nemirovski (Georgia Institute of Technology, USA)

The data in real-life optimization problems usually are uncertain; that is, not known exactly when the problem is to be solved. Examples demonstrate that even small perturbations of uncertain data can make the optimal solution corresponding to the *nominal* data values heavily infeasible; and thus, practically meaningless. Robust Optimization methodology proposed in mid-90s and rapidly developing since then is aimed at building *robust optimal* solutions (those remaining feasible for all realizations of the data from a given uncertainty set), and optimizing under this restriction a given objective function.

In the talk, we outline the basic concepts of RO in the context of uncertain *well-structured* convex optimization problems (linear, conic quadratic and semi-definite programming), with emphasis on recent extensions of the RO paradigm and on the central issue of computational tractability/building tight tractable approximations of the robust counterparts of uncertain problems. We intend also to discuss recent links between RO and Chance Constrained Stochastic Programming, a more traditional way to handle data uncertainty in Optimization.

IC/IT4558: *Chaotic itinerancy reality in brain dynamics*

Ichiro Tsuda (Hokkaido University, Japan)

Motivated by the recent finding of transitory dynamics on the brain activity, we have studied high-dimensional chaotic dynamical systems related to neural systems. In the first part of the talk, we would like to focus on chaotic itinerancy as a key concept for understanding the observed transitory phenomena. In the second part, we provide a mathematical model for the hippocampus in order to clarify the mechanism of the formation of episodic memory. The model produces transitory dynamics which is similar to what observed in the hippocampus. The detailed numerical studies clarified that the transitory dynamics can be represented by chaotic itinerancy. Furthermore, the model predicts that the time series in the transitory dynamics can be encoded by Cantor sets in the state space of neurons. We show that this prediction has been proven in the experiments on the hippocampus.

IC/IT4851: *Design, analysis and application of optimal PDE solvers*

Jinchao Xu (Pennsylvania State University, USA)

This talk is devoted to optimized numerical methods for partial differential equations (PDEs) by an integrated design and application of discretization, grid adaptation and algebraic solution of the resulting discrete systems. After giving a general perspective, a number of recent results will be presented to demonstrate that many linear and nonlinear PDEs (such as model equations for electromagnetic, complex fluids and fuel cells) can be practically solved with (nearly) optimal computational complexity.

Johnson–Segalman and other mathematical models for non-Newtonian fluids are among the examples to be discussed. A sophisticated finite element scheme (recently developed jointly with Y. Lee) will be reported for these nonlinear systems. This scheme is stable for any size of the Weissenberg number (while almost all other existing discretizations suffer from the well-known High Weissenberg Number Problem), and, at each time step, its discretized system is reduced to one linear system and a number of independent ODEs that can be solved in parallel.

Algebraic systems resulting from such properly discretized PDEs can be effectively solved by multilevel methods based on subspace correction and auxiliary space precondition. By using new convergence criteria and estimates (from joint works with L. Zikatanov, J. Wu and Y. Lee) for these methods, robust algorithms are developed for a large class of singular, nearly singular and indefinite system of equations. The method of subspace correction is shown to be uniformly convergent for nearly singular system if the underlying near-null space can be linearly represented by its intersection with all relevant subspaces. The method of auxiliary space preconditioning is applied (in a recent joint work with R. Hiptmair) to construct optimal preconditioners for $H(\mathrm{curl})$ and $H(\mathrm{div})$ systems based on user-friendly solvers (such as algebraic multigrid methods) for Poisson-like equations.

IC/IT4523: *Topology optimization of structures*

Grégoire Allaire (École Polytechnique Palaiseau, France)

The typical problem of structural optimization is to find the *best* structure which is, at the same time, of minimal weight and of maximum strength or which performs a desired deformation. In this context I will present the combination of the classical shape derivative and of the level-set method for front propagation. This method has been implemented in two and three space dimensions for models of linear or non-linear elasticity and for various objective functions and constraints on the perimeter. It has also been coupled with the bubble or topological gradient method which is designed for introducing new holes in the optimization process. Since the level set method is known to easily handle boundary propagation with topological changes, the resulting numerical algorithm is very efficient for topology optimization. It can escape from local minima in

a given topological class of shapes and the resulting optimal design is largely independent of the initial guess. I will discuss various applications and numerical examples.

IC/IT4958: *Contact problems in solid mechanics*
Michel Fortin (Université Laval, Canada)

Contact problems are industrially important and present a number of difficult mathematical issues: they are free-boundary problems, which are described by a quasi-variational inequality. We shall address some issues related to these problems.

- Discretisation implies a mixed finite element analysis. Stability is obtained in weak spaces, which implies trouble in numerical computation. We shall present some choices of elements, which are suitable for three-dimensional computation.
- Well-posedness of the classical Coulomb's law is not clear: the frictional threshold depends on a variable for which point values are far from being defined.

We shall also present an algorithm for the numerical solution, based on a conjugate gradient method with projection. It will be employed to solve a sequence of Tresca's problems with an external iteration on the threshold. As we shall discuss, use on the Coulomb's cone induces a loss of symmetry, which impairs the convergence of gradient methods.

Real problems also imply geometrical difficulties, especially when two deformable bodies get in contact. Some of these problems will be treated correctly but other ones only through heuristic considerations. Finally, mesh adaptation appears to be an important technique to provide accurate and usable computations. Numerical results will also be presented.

IC/IT4368: *Numerical methods for nonlinear elliptic problems*
Roland Glowinski (University of Houston, USA)

The main goal of this lecture is to address the *numerical solution* of several classes of *nonlinear elliptic problems*. This includes *nonlinear eigenvalue problems* such as

$$-\Delta u = \lambda u^3 \tag{1}$$

and *fully nonlinear elliptic equations* of the Monge–Ampère type. It will be shown, that by well chosen combinations of finite element approximations, least-squares formulations and operator-splitting methods one can build a methodology which is robust and flexible, and which provides for some of the problems under consideration (the elliptic Monge–Ampère equation for example) an alternative to the methods based on the concept of viscosity solutions. Actually, it will be shown, via an appropriate transformation, that some of the least-squares methods to be discussed are viscosity solutions but in a sense different from Crandall and P.L. Lions. The results of various numerical experiments will be presented. They concern, in particular, the solution of Monge–Ampère type equations and the computational investigation of some examples of the above equation.

IC/IT4970: *Asymptotic solutions of Hamilton–Jacobi equations for large time and related topics*
Hitoshi Ishii (Waseda University, Japan)

I will discuss recent developments on the study of the asymptotic behavior, as $t \to \infty$, of solutions $u = u(x,t)$ of Hamilton–Jacobi (HJ for short) equations $\partial u/\partial t + H(x, Du(x,t)) = 0$ in $\mathbb{R}^n \times (0,\infty)$, where $H : \mathbb{R}^n \times \mathbb{R}^n \to \mathbb{R}$ is a continuous function and $Du = (\partial u/\partial x_1, ..., \partial u/\partial x_n)$. Hamilton–Jacobi equations are basic equations in the dynamic programming approach to optimal control and differential games. S. N. Kruzkov in the 60s and P.-L. Lions and G. Barles in the 80s initiated the study of the large-time behavior of solutions of HJ equations.

In the last decade many authors, including G. Namah, J.-M. Roquejoffre, A. Fathi, G. Barles, P. E. Souganidis, A. Davini, A. Siconolfi, Y. Fujita, P. Loreti, ..., investigated the aymptotic behavior of large-time solutions of HJ equations under the influences of or interaction with weak KAM theory as it was developed by A. Fathi and A. Siconolfi among others. My talk will cover:

(i) the additive eigenvalue problem (ergodic control problem) for HJ equations;
(ii) the weak KAM theory and representation theorems for solutions of HJ equations;
(iii) the asymptotic behavior of solutions of HJ equations.

IC/IT4516: *Hyperbolic conservation laws: past and future*
Barbara Keyfitz (Fields Institute, Canada)

The field of conservation laws (quasilinear hyperbolic partial differential equations) has captured the attention of mathematics researchers, computational fluid dynamicists, and modelers of physical and engineering phenomena for over 70 years. This talk will survey some of the power, and some of the limitations, of the conservation law approach to modeling. It will also expound some of the major achievements in establishing a mathematical theory, and discuss why theoretical advances have been so slow, and why so much still seems to remain out of reach. Finally, I will describe recent work of a number of people on establishing mathematical properties of shock reflection phenomena.

IC/IT4552: *Mathematics sets the molecular world in motion*
Christof Schütte (Freie Universität Berlin, Germany)

Since several decades Molecular Dynamics (MD) has been a field of world-wide research activities. Until recently it has mainly been focussed towards the prediction of the minimal-energy geometry of a molecule and the computation of statistical quantities like transport coefficients or free energies. Progress in molecular biophysics and molecular chemistry, as well as in materials science, has made it clear that the effective dynamical behavior of a molecular system is essential for its functions/properties. However, available experimental techniques do not suffice to understand the effective dynamics in appropriate detail. In addition, direct MD simulation of the effective dynamics of many molecular systems is infeasible even on the fastest computers of today and the foreseeable future, since the typical timescale of interest is many (typically more than 10) orders of magnitude larger than the fastest scales that have to be resolved.

Recent progress in mathematical modelling, in combination with novel simulation strategies and new experimental techniques, has brought us much closer to solving this problem. The talk will introduce the mathematical background of the problem, explain what is meant by effective dynamics, define the mathematical objects that are required to appropriately understand it (almost invariant/metastable sets, transition rates, transition paths), present algorithmic concepts for their efficient computation, and illustrate the resulting insight into the effective dynamics of some molecular systems of biological interest.

IC/IT4122: *Controllability and observability: from ODEs to quasi-linear hyperbolic systems*

Tatsien Li (Fudan University, PR China)

By means of the semi-global classical solution, a simple and direct constructive method is presented to give a complete result with applications on the exact boundary controllability and the exact boundary observability for 1-D quasilinear hyperbolic systems with general nonlinear boundary conditions.

IC/IT5010: *Radar imaging*

Margaret Cheney (Rensselaer Polytechnic Institute, USA)

Synthetic-aperture radar imaging is a technology that has been developed, very successfully, within the engineering community during the last 50 years. Radar systems now make beautiful and very useful images of our earth and other planets. One of the key components of this impressive technology is mathematics, and many of the open problems are mathematical ones.

This lecture will explain, from first principles, the basics of radar and some of the mathematics involved in producing high-resolution radar images. The talk will conclude with a quick survey of some of the specific problems on which more mathematical work is needed

01: Computing

Computing, Minisymposia

IC/MP55/015: Applied analysis meets scientific computing.

Organiser: Laurent Demanet (California Institute of Technology, USA)
Co-organiser: Lexing Ying (University of Texas at Austin, USA)

This minisymposium will focus on some recent ideas for efficient computation of the wave and Helmholtz equations. These ideas have in common that they aim at high, controlled accuracy using a minimum number of degrees of freedom through adequate representations. 1) A first research avenue is the multipole expansion for convolution with the Helmholtz kernel, which allows to solve the second-kind boundary integral equations for surface scattering with remarkable speed and accuracy. 2) A second research avenue are the geometric multiscale expansions of wave propagators inspired by the second dyadic decomposition. These methods include curvelets, wave atoms, and symbol separation. For the wave equation, they offset the need for traditional timestepping through manipulations of operators in compressed form. For related oscillatory integrals, they offer near-optimal complexity algorithms. 3) A third research avenue is computation of eigenfunctions of the Laplacian in bounded domains through superposition of Helmholtz kernels and generalized Green's identities. This alternative approach currently yields the most accurate codes for quantum billiards and waves inside complicated cavities. We hope this minisymposium will help highlight the similarities and complementarity of these three approaches.

Operator-based wave computations. **Laurent Demanet** (California Institute of Technology, USA) IC/MT2556/010

This talk presents a new algorithm for linear hyperbolic PDE with smooth coefficients, based on a formulation of the Green's function that uses Fourier integral operators. The computation mostly involves manipulations of operators in compressed form, which can be done in complexity essentially independent of the resolution of the initial data. This stratgey becomes advantageous in regimes where the wavefields are very oscillatory. Operators are compressed and manipulated using techniques such as phase-space partitionings, traveltime computations via the phase-flow method, low rank matrix approximations via random sampling, special quadratures that exploit the geometry of the canonical relation, etc. This is joint work with Lexing Ying.

Combining finite differences/finite elements with geometrical wave propagation in 1D. **Christiaan Stolk** (Universiteit Twente, The Netherlands) IC/MT3000/010

We show that the initial value problem for a strictly-hyperbolic partial differential equation on the circle can be solved at cost $O(N)$. To obtain this, the equation is approximately decoupled, into first order equations that can be solved using the method of characteristics. The error satisfies an ODE in a function space, that is of the form $du/dt = R(t)u$, with $R(t)$ a bounded operator. With an appropriately designed scheme, using time-steps longer than allowed by the CFL condition in FD/FE schemes, this leads to the stated complexity. The main assumption is that the coefficients in the PDE vary on a longer scale than the initial values. An implementation of the new method performs comparable or better than standard fourth order finite differences in examples of this kind.

Global approximation methods for high-frequency eigenmodes. **Alex Barnett** (Dartmouth College, USA), Timo Betcke (University of Manchester, UK) IC/MT3489/010

The efficient computation of eigenmodes has applications to both engineering problems (acoustics, optical cavities) and more fundamental problems of mathematical physics (quantum chaos, spectral geometry, automorphic forms). The interesting case of high-frequency (system is many wavelengths across) remains numerically challenging. The use of global basis approximation by Helmholtz solutions, combined with matching on the boundary, has undergone a revival due to a recent convergence of ideas from the physics and numerical analysis communities. I will present various global basis sets, discuss the mode of failure of plane-wave bases, and demonstrate the success of fundamental solutions (with origins placed outside the domain) in a large class of 2D domains. The latter basis achieves high accuracy with as few as 3 degrees of freedom per wavelength on the boundary. I present some open questions regarding the convergence rate of such bases. Finally I present a further advantage of such methods: that acceleration (scaling) methods exist which allow a further increase in speed by $O(k)$, where k is the wavenumber. Some of this talk covers joint work with T. Betcke.

A fast phase-space method for computing creeping waves. **Olof Runborg** (Kungliga Tekniska högskolan, Sweden) IC/MT4979/010

Creeping rays can give an important contribution to the solution of medium to high frequency scattering problems. They are generated at the shadowlines of the illuminated scatterer and propagate along geodesics on the scatterer surface, continuously shedding diffracted rays in their tangential direction. We show how the ray propagation problem can be formulated as a partial differential equation (PDE) in a three-dimensional phase space. The PDE solution give information about all possible creeping rays. Computationally the cost of solving the PDE is less than tracing all rays individually. We show numerical results and an application to monostatic radar cross section problems where creeping rays from all illumination angles must be computed.

IC/MP162/015: Microlocal analysis meets scientific computing.

Organiser: Laurent Demanet (California Institute of Technology, USA)
Co-organiser: Lexing Ying (University of Texas at Austin, USA)

Various theories and algorithms have recently been developed to better exploit the microlocal nature of wave-based or tomographic inverse problems. Microlocal analysis is the mathematical study of singularities of functions in phase-space, and how those singularities are transformed by linear operators and PDE. For example, the problem of recovery of the index of refraction of a medium from high-frequency wave measurements is generally convexified and much simplified when only the singularities are studied. The objects to compute in this setting are often generalized Radon transforms or Fourier integral operators. In contrast to traditional PDE or integral equation solvers, microlocal numerical methods consider the map-

ping of singularities as the entity of interest (the canonical relation itself) and discretize it either 1. through direct sampling, or 2. through phase-space tilings, or 3. through diffeomorphisms. The emphasis of this minisymposium will be on inverse problems and on the above-mentioned three algorithms for solving them; with applications to imaging of singularities in reflection seismology, and rendering of hard shadows due to occluders in computer graphics.

Microlocal computation of hard shadows. **Gabriel Peyré** (Université de Paris–Dauphine, France) IC/MT2870/010

Accurately rendering hard shadows (sharp luminosity constrasts) is one of the main challenges of computing illumination of 3D scenes in animated movies. The difficulty is due to the high-dimensionality and the singularity of the integral kernel of the so-called radiance equation governing shadow forming. Contemporary rendering methods are based on Fourier or Monte Carlo methods that are completely oblivious to the geometry of this integral kernel. In joint work with Laurent Demanet, we propose a different viewpoint: the map linking the light source to the shadow boundary is very well expressed, in the language of microlocal analysis, as a relation between wavefronts in phase-space. We call it the "light-shadow relation". Its explicit computation is an integral part of an envisioned algorithm for computing hard shadows much more efficiently than previously. This microlocal viewpoint also ties in with sparse wave packet (curvelet, bandelet) techniques for representing the radiance integral operator. We hope to report on preliminary numerical results.

Travel-time tomography. **Gunther Uhlmann** (University of Washington, USA) IC/MT3259/010

We consider the inverse problem of determining the anisotropic index of refraction of a medium by measuring the travel times of waves going through the medium. In mathematical terms this consists in determining the Riemannian metric of a Riemannian manifold with boundary from its lengths of geodesics (i.e multiple arrival times.)

We will also consider a very related problem in phase space. Assume that we know for every geodesic going through the medium its point of entrance and direction of entrance and its point of exit and direction of exit. This information is encoded in the scattering relation. Can we recover the Riemannian metric (i.e. index of refraction) from the scattering relation?

A multi-scale approach to evolution equations with applications in wave-equation imaging. **Maarten de Hoop** (Purdue University, USA) IC/MT3262/010

Downward continuation based imaging and wave-equation reflection tomography can essentially be expressed in terms of solving particular evolution equations. The underlying model describes the single scattering of waves in a background medium. Here, we are concerned with developing a method that admits background media of limited smoothness, which leads to evolution equations generated by certain pseudodifferential operators. We develop a multi-scale approach to solving such evolution equations, while making use of solution representations based on wavepackets or a (co)frame of curvelets and a (curvelet-curvelet) scattering series. We discuss results concerning the 'concentration' of curvelets. We also discuss computational aspects of the method that leads us to an approach that departs from the use of (co)frames.

Joint research with H. Smith (UW), G. Uhlmann (UW), F. Andersson (Lund).

Fast directional multilevel computation for problems with oscillatory kernels. **Lexing Ying** (University of Texas at Austin, USA) IC/MT4799/010

We introduce a new directional multilevel algorithm for solving the N-body or N-point problems with highly oscillatory kernels. These problems often result from the boundary integral formulations of scattering problems and are difficult due to the oscillatory nature of the kernel and the non-uniformity of the particle distribution.

We address the problem by first proving that the interaction between a ball of radius r and a well-separated region has an approximate low rank representation, as long as the well-separated region belongs to a cone with a spanning angle of $O(1/r)$ and is at least $O(r^2)$ away from from the ball. We then propose an efficient and accurate procedure which utilizes random sampling to generate such a separated, low rank representation. Based on the resulting representations, our new algorithm organizes the high frequency far field computation in a multidirectional and multiscale strategy to achieve maximum efficiency.

The algorithm performs well on a large group of highly oscillatory kernels. Assuming that the points are sampled from a two dimensional surface, our algorithm has provably $O(N \log N)$ complexity for any given accuracy. We also provide numerical results to demonstrate these properties.

IC/MP164/015: High-dimensional analysis meets scientific computing.

Organiser: Laurent Demanet (California Institute of Technology, USA)
Co-organiser: Lexing Ying (University of Texas at Austin, USA)

This minisymposium will focus on scientific computing in high dimensions. The attainable size of simulations using textbook methods, when used in $\mathbb{R}^d$, with d large, typically scales at best like the $1/d$-th power of computer performance. While this phenomenon is already a problem for physics in $\mathbb{R}^3$, truly high-dimensional problems include the multiparticle Schrödinger equation, reflection seismology with its high-dimensional acquisition manifolds, and kinetic gas theories in phase-space. Fortunately, adapted techniques have emerged over the past few years to better redefine what computations need to be done and what data need to be stored for solving high-dimensional PDE.

(1) One of these methods is sparse grids, where boundedness of the mixed partial derivatives is used to cut down the complexity of sampling;

(2) another such method is H-matrices, where partitioned low-rank representations are available for kernels of large classes of integral equations;

(3) finally, separated representations generalize the notion of low rank and SVD to tensors of order higher than 2.

All these methods, and others, should be discussed in this minisymposium.

$\mathcal{H}^2$-matrices. **Steffen Börm** (Max-Planck-Institut Leipzig, Germany) IC/MT2709/010

Hierarchical matrices are data-sparse representations of dense matrices which make it possible to perform operations like matrix-vector multiplication, matrix addition, multiplication or inversion in almost linear complexity. Due to this property, hierarchical matrices can be used to construct preconditioners for integral or partial differential equations and to solve problems from control theory.

$\mathcal{H}^2$-matrices combine the basic ideas of hierarchical matrices with those of multilevel methods in order to perform certain operations in "true" linear complexity.

The basic idea is that matrix blocks corresponding to domains which are far do not contain a singularity can be represented in the factorized form $VSW^\top$, where the matrices V and W describe the basis in which the block is expressed and S contains the corresponding coefficients. The key problem of $\mathcal{H}^2$-matrix arithmetics is the construction of suitable bases. For integral equations, it can be solved by using polynomial interpolation or multipole expansion, possibly with subsequent algebraic optimization. The same optimization techniques can also be applied to general matrices.

In the case of integral operators, $\mathcal{H}^2$-matrices can be interpreted as efficient representations of the $(2d)$-dimensional kernel function. Although typical kernel functions do not satisfy the standard regularity assumptions of sparse grid or Kronecker tensor techniques, they can still be approximated by $\mathcal{H}^2$-matrices corresponding to block-tensor decomposition of the computational domain.

Adaptive wavelet algorithms for PDEs on product domains. **Rob Stevenson** (Universiteit Utrecht, The Netherlands), Christoph Schwab (ETH Zürich, Switzerland) IC/MT2745/010

With standard isotropic approximation by (piecewise) polynomials of fixed order in a domain $D \subset \mathbb{R}^d$, the convergence rate in terms of the number N of degrees of freedom is inversely proportional to the space dimension d. This so-called *curse of dimensionality* can be circumvented by applying sparse tensor product approximation, when certain higher order mixed derivatives of the approximated function happen to be bounded in L_2. Solutions of PDEs, however, satisfy this condition in special situations only.

Considering best N-term approximation from tensor product wavelet bases, in [*Constr. Approx.*, 24 (1) (2006), 49-70], Nitsche showed that the above regularity constraint can be dramatically reduced to a condition that is satisfied by the solutions of (elliptic) PDEs. Adaptive wavelet algorithms realize convergence rates as that of best N-term approximations in linear complexity *assuming* that the infinite stiffness matrix of the operator with respect to such a basis is highly compressible. Applying piecewise smooth wavelets, we verify this compressibility for general, non-separable elliptic PDEs in tensor domains, with that demonstrating optimality of the adaptive wavelet algorithms. We hope to be able to illustrate our theoretical considerations by numerical results.

Hierarchical low-Krönecker-rank approximation. **Lars Grasedyck** (Max-Planck-Institut Leipzig, Germany) IC/MT3338/010

The treatment of high-dimensional PDEs is in particular challenging because of the curse of dimension, i.e., that the dimension d enters the complexity exponentially for naive approaches. One method to avoid the curse is to use efficient compressions on full tensor grids. Even though the full space contains $\mathcal{O}(N^d)$ degrees of freedom, associated grid functions can be approximated with much less data. The idea is to approximate discrete vectors x in this space by low Kronecker rank $k \ll N^d$:

$$x_{i_1,\dots,i_d} \approx \sum_{\nu=1}^{k} \prod_{j=1}^{d} y_{\nu,i_j} =: y_{i_1,\dots,i_d}, \qquad i_j \in \{1,\dots,N\}.$$

The Kronecker rank k vector y is represented by kdN data, i.e. with a complexity that scales multi-linearly in the dimension d, the number of mesh points N per axis and the Kronecker rank k.

In this talk we will focus on the question how one can compute with vectors in the compressed low Kronecker rank representation. We consider on the one hand side a high-dimensional PDE where the right-hand side has low Kronecker rank. There, we can prove that the solution allows for a low Kronecker rank approximation and we can derive explicit formulae for the solution in this format. The format involves matrix exponentials which are treated by hierarchical matrix techniques in almost linear complexity.

On the other hand we present methods for the efficient truncation from a larger Kronecker rank K to a smaller Kronecker rank $k < K$. This truncation then allows the use of iterative solvers for systems where the inverse does not allow for an explicit formula.

Preliminary results on approximating a wavefunction as an unconstrained sum of Slater determinants. **Gregory Beylkin** (University of Colorado at Boulder, USA), Martin Mohlenkamp (Ohio University, USA), Fernando Pérez (University of Colorado at Boulder, USA) IC/MT5044/010

A multiparticle wavefunction, which is a solution of the multiparticle Schrödinger equation, satisfies antisymmetry condition, thus making it natural to approximate it as a sum of Slater determinants. Many current methods do so but, in addition, they impose structural constraints on the Slater determinants, such as orthogonality between orbitals or a particular excitation pattern. By removing these constraints, we hope to obtain much more efficient expansions.

We use an integral formulation of the problem, a Green's function iteration, and a fitting procedure based on the computational paradigm of separated representations. For constructing and solving a matrix-integral system of equations derived from antisymmetric inner products, we develop new algorithms with computational complexity competitive with current methods.

We describe preliminary numerical results and make some observations.

IC/MP283/010: Parallel Matlab.

Organiser: John Gilbert (University of California, Santa Barbara, USA)

As the computational demands of scientific modeling and simulation rise, and the cost of parallel computing hardware drops, more and more computational scientists wish to use parallel computation. Matlab is an extremely popular language and interactive environment for doing computational science on workstations. There is a clear motivation to make it possible to run Matlab programs on very large problems using parallel computers.

The speakers in this minisymposium will describe a number of projects that are building parallel implementations of the Matlab language. Cleve Moler, Chief Scientist of The MathWorks and the developer of Matlab, will describe his work on Parallel Matlab. Alan Edelman of MIT and Interactive Supercomputing Inc. will present Star-P, an interactive system that allows computational scientists to use the Matlab language to program parallel supercomputers and commodity clusters. Ashok

Krishnamurthy (Ohio State University and the Ohio Supercomputing Center) will discuss the application of several parallel implementations of Matlab in image processing. John Gilbert (UC Santa Barbara) will describe a set of tools for computing on large graphs that is based on the parallel sparse array implementations in Matlab and Star-P.

The star-P parallel platform for use with Matlab®, Python, and symbolic software. **Alan Edelman** (Massachusetts Institute of Technology, USA) IC/MT4196/010

The Star-P parallel platform allows Matlab users, and users of other languages, to program in parallel in an open easy to use environment. We will show the details underlying the system and what users need to know to write effetive parallel codes.

Parallel Matlab. **Cleve Moler** (The MathWorks, Inc., USA) IC/MT1621/010

In the MathWorks design of Parallel MATLAB, each node of a multiprocessor computing environment executes a program written in the MATLAB programming language. Key features of the system include parallel for loops, distributed arrays, and global reductions. We will describe these features in more detail and demonstrate them with several examples. Our motto is "Think Matrices, Not Messages".

Performance metrics and measurements for PGAS Matlab implementations. **Ashok Krishnamurthy** (Ohio Supercomputer Center, USA) IC/MT4212/010

Matlab is a widely popular scientific programming tool. As applications written in Matlab have required larger data sets and more computational power, parallel extensions for Matlab have emerged. One notable category of parallel Matlab extensions are those that provide partitioned global address space (PGAS) support. PGAS is a programming model in which an application is viewed as a collection of concurrent threads that can communicate with one another via a globally shared data space. PGAS provides a high-level abstraction for parallel programming and pairs quite naturally with the array-based notation of Matlab.

However, it is not enough to merely write parallel code; developers want to create efficient parallel code. In that regard, a tradeoff exists between the abstractions provided by the PGAS model and the specifics of the architecture impacting the execution. A number of recent efforts in PGAS performance metrics and measurements such as the global address space performance (GASP) tool show promise in providing performance feedback to developers.

In this paper, we consider performance measurements and metrics for two PGAS versions for Matlab: MathWorksŠ proprietary Distributed Computing Toolbox/Distributed Computing Engine (DCT/DCE) and an open source solution known as pMatlab+bcMPI. We describe a relevant set of PGAS metrics and describe the implementation of a set of common performance measurements. We ran a number of benchmarks relevant to the signal processing domain with each version on a cluster and present results correlating the metrics with the actual parallel efficiency. We feel that the data validate the utility of these metrics in tuning applications for improved parallel efficiency.

A high-performance interactive environment for exploring large graphs. **John Gilbert** (University of California, Santa Barbara, USA) IC/MT3239/010

High-performance computing is being used to understand large data sets that are combinatorial rather than numerical in nature, in applications as diverse as sparse matrices, knowledge discovery, machine learning, search and information retrieval, and computational biology.

Compared to numerical supercomputing, the field of high-performance combinatorial computing is in its infancy. How can combinatorial methods be used by people who are not experts in discrete mathematics? How can supercomputers be used by people who need to explore huge discrete data sets interactively?

We are using a parallel dialect of Matlab to build a flexible, scalable interactive environment for high-performance computation on discrete structures that will be used both as a rapid-prototyping tool for exploring and experimenting with different approaches to analysis, and as a scalable system for performing analysis on real, dynamic, discrete data.

IC/MP263/011: Math on the web: content development and implementation.

Organiser: Daniel Lozier (National Institute of Standards & Technology, USA)
Co-organiser: Abdou Youssef (The George Washington University, USA)
Co-organiser: Bruce Miller (NIST, USA)

Since the advent of the Web, various projects and activities have been undertaken worldwide to put math on the Web. Moving beyond the assembling of digitized collections of documents into databases with some basic text-search capabilities, recent efforts have focused on: 1. creating standards and software tools for math-content development; 2. developing feature-rich digital libraries of mathematics; and 3. applying the tools and digital libraries to more effective math education and the advancement of math research. For example, XML-based math representation languages for the Web have been developed, most notably OpenMath and MathML, along with major extensions such as OMDOC. Various LaTeX-to-HTML and LaTeX-to-XML conversion tools, such as LaTeXML, have been created, and leading computer algebra systems now provide features for exporting content to MathML. Slated to be released soon is the Digital Library of Mathematical Functions (DLMF), which is a library of thoroughly validated, highly-robust contents, represented in LaTeX and XML, and designed for use in advanced applications of special functions in science, engineering, and other technical disciplines. The DLMF also has a new math-enabled search system for quick and easy access not only to text but also to equations and math expressions.

The focus of this minisymposium is to present to mathematicians and users of mathematics a carefully selected cross-section of the activities, tools, and current practices of putting math on the Web, describe their benefits, and begin to outline a vision of what math on the Web (MOW) will be. The objectives are threefold:

(1) to inform the community at large of the state of the art of MOW technology;
(2) to share with current and future MOW designers and developers the lessons learned from ongoing projects; and
(3) to identify feasible and useful future directions that MOW needs to follow.

Eight of the top leaders and advocates of the MOW field will present talks at this minisymposium.

Utilizing the DLMF in scientific research. **Daniel Lozier** (National Institute of Standards & Technology, USA) IC/MT4971/011

The NIST Digital Library of Mathematical Functions (DLMF) is to be the Web and hard copy successor to the well-known and highly successful NBS Handbook of Mathematical Functions, edited by M. Abramowitz and I. A. Stegun. This talk, by the DLMF General Editor, describes ways in which the Web interface to the mathematical database of the DLMF augments the traditional manner of access to scientific reference information.

Lessons from the trenches: a survey of approaches for large-scale projects. **Robert Miner** (Design Science, Inc., USA) IC/MT1510/011

Large-scale projects play an important role in today's Math on the Web landscape. Technical content is continually being published to the Web in many contexts, ranging from individual educators posting course notes to major science publishers producing online journals. However, for most people, the bulk of useful technical material tends to be in large-scale, ongoing, actively curated collections.

One obvious reason that a large proportion of the most valuable technical content resides in large collections is that publishing technical content is technically challenging. Just as with print, authoring technical documents for the Web requires special software and expertise. Similarly, available display options within Web browsers either involve significant compromise in quality, or a significant increase in technical complexity. Between authoring and display, the workflow processes that ensure high-quality, high-functionality documents add more complexity still, but they also have potential to add value beyond the reach of most small projects. All these factors favor large-scale, ongoing operations where technical expertise can be concentrated and leveraged.

Of the leading large-scale repositories of technical content, most are comparatively old and established. Their technology platforms have evolved alongside XML and Web technology, and now reflect the state of the art. Their production processes have similarly matured. Unsurprisingly, over time, a small number of strategies have emerged as viable choices for the major stages of any Math-on-the-Web workflow: authoring, intermediate processing and display. In this talk, we will survey the strategies employed by a number of leading Math-on-the-Web projects such as Wikipedia, the arXiv, Connexions, the World Math Digital Library, a number of commercial and society publishers, and assorted others.

Extending the Reference Web *using modern TEXniques.* **Ross Moore** (Macquarie University, Australia) IC/MT4972/011

Having ready access to the metadata for scientific papers is important in enabling interested researchers to locate work done by others that is relevant to their own studies. Modern TEX systems can do a lot more than just produce a printable version of a paper suitable for publication. In this talk I will show examples of PDFs of mathematical papers for which the same TEX run produces metadata files in different formats (such as BibTEX, XML, RSS) which are included within the PDF files as attachments. Also the TEX run composes a web-page that displays the metadata, including all the references (á la "Reference Web" recommendations), to fit into a web-site for all articles within a volume issue of the particular journal. This page includes hyperlinks to the MathSciNet database entry for each cited reference, whenever these exist.

One particular advantage of distributing metadata in this way, is that the possibility for mis-spelling (e.g., of the author's name) is reduced, since it has been generated from the same source information used to typeset the article itself. Furthermore, obtaining the MathSciNet entries for cited references is programmed to be done automatically as part of the TEX job. This feature is not 100% reliable, but is easily supplemented by manual searching, and can be suppressed if desired. Other PDF navigation features and effects are included to make the online reading experience much easier; e.g., on a laptop, and for when electronic paper becomes a reality. Among these features are bookmarks (including math-symbols) and hyperlinks to significant parts of the article, moveable pop-up figures, back-references to citations, and use of colour for headings, equation numbers, theorems, definitions, remarks, and such-like.

Discussion of the advantages of these features in other contexts is encouraged. If time permits, methods used to construct the CD and website of abstracts for this ICIAM-07 congress may also be examined.

Content-level mathematics: its usage in learning on the web. **Paul Libbrecht** (DFKI GmbH and Universität des Saarlandes, Germany) IC/MT2439/011

Encoding of mathematical objects and documents can be done at three levels: the presentation level, with TeX or MathML as examples, encodes such constructs as paragraphs, exponents, or rows of operator-symbols and identifiers; the semantic level provides structure to encode the full mathematical meaning of each statement, proof, and expression, hence includes all formal and logical details in a proof or a statement.

content-level mathematics representations encode parts of mathematical documents as a structure of meaningful fragments, such as definitions or motivations and allows for textual parts as well as mathematical formulae using applications, bindings, and named symbols. Mathematical documents at the content-level are much easier to encode and exchange than at the semantic level and they are more interoperable and reusable than presentation-level representations since parts are defined with their mathematical roles.

For many applications the content-level suffices for reuse and interoperability since the additional proof information in which calculus and under which assumptions a theorem has been proved may not be relevant for the application.

The OMDoc language is a content-level encoding, including OpenMath. The ActiveMath learning environment puts this encoding in action, providing strong services which use the knowledge structure encoded.

We shall present an overview of the usage of content-level mathematics as it currently works in ActiveMath, e.g., the cross media formulae presentation, the ability to copy-and-paste formulae, the domain-knowledge structuring the learner-modelling and pedagogically founded content-selection...

Our approach to input of content-level-mathematics will be described. At the heart of the challenges lies the extensibility of the mathematical ontology built by content-level-mathematics. We promote the freedom of authors to define new symbols and concepts as opposed to a central ontology engineering. This brings all kind of problems e.g when the domain-knowledge for the student model is generated from them. These problems are natural and uncover inconsistencies in content which have to be recovered in the authoring process. This freedom also challenges the interoperability with external mathematical systems for which we explore solutions' avenues.

IC/MP263/011: **Math on the web: content development and implementation.** #2
Organiser: Daniel Lozier (National Institute of Standards & Technology, USA)
Co-organiser: Abdou Youssef (The George Washington University, USA)
Co-organiser: Bruce Miller (NIST, USA)

(For abstract, see session #1 above.)

Language technologies for semantic markup in mathematics. **Olga Caprotti** (University of Helsinki, Finland) IC/MT2925/011

In this talk we will report the recent progress obtained in the frame of the Web Advanced Learning Technologies project in applying state of the art language technologies to semantic markup of mathematics for automatically producing renderings of mathematical content in a variety of languages. The intended application of this work is the area of computer assisted assessment and testing in mathematics where can be used to produce, for instance, standardized entry examinations for perspective students to be used independently of country and language. A similar approach can be developed for any situation in which it is possible to identify a specific mathematical jargon.

Respecting implicit semantics in mathematical markup. **Stephen Watt** (University of Western Ontario, Canada) IC/MT3554/011

We present a new strategy for conversion between TEX mathematical expressions and MathML. Previous efforts have attempted either superficial high level transliteration or full execution of TEX. We observe that important semantic concepts are often present in the source markup in the form of macro applications. Our approach is unique in retaining this implicit semantic information as the documents are translated. The translator output may be used immediately by applications, or can be adopted as *replacement source* for on-going work. Our implementation allows control over which macros are expanded and which are mapped at a semantic level.

The principal contributions of this work are:

- A new approach to TEX/MathML translation that conserves and exploits implicit semantics.
- An architecture that allows new representations of semantic information to be associated with existing documents (e.g., association of OpenMath definitions to existing LATEX documents).
- Useful converters from TEX math to MathML and MathML to TEX, and an examination of issues that arise in their implementation.

Creating webs of math using LATEX. **Bruce Miller** (NIST, USA) IC/MT2597/011

How can authors and editors create mathematical content targeted for print and the web, and perhaps uses unforeseen, in a way that takes fullest advantage of each media's capabilities? We will flesh out this question by discussing and contrasting the capabilities and needs of each medium as well as the apparent conflicts. We will highlight some of the possibilities enabled by the web that are unique to mathematical material. After giving a brief overview of the possible answers to the question, we will focus on one tool, LATEXML, that is being used in the Digital Library of Mathematical Functions (DLMF) project. LATEXML converts LATEX sources to an XML format that closely mimics the LATEX document structure and which is easily converted to HTML, images, MathML and other formats. Using LATEX helps solve the print issue. By mimicking LATEX's structure, it helps avoid loosing the author's semantic intent. More interesting, by leveraging TEX's macro capability, on the one hand, and LATEXML's extensibility, on the other, it allows authors to enhance the semantic content, meta-information and document structure to whatever extent is needed. We will illustrate with examples from the DLMF.

Recent advances in Math Search. **Abdou Youssef** (The George Washington University, USA) IC/MT1311/011

As Web repositories and digital libraries of mathematical contents proliferate, one key support service is math-aware search. A math-aware search system should allow users to enter math queries that involve not only text keywords, but also mathematical expressions, expression-fragments, and various mathematical symbols. The system should also *understand* the math contents: symbols and structures, and thus be able to match math queries to math contents.

Several research projects for developing math search techniques and systems have been undertaken in North America and Europe, and even some search systems have been deployed or about to be completed and put into operation. A few of the systems are special purpose, such as table lookups or formal-math search, while others are roughly general purpose, tailored to general math-expression search.

This talk will address the advances made so far in math search. The different approaches will be outlined, a preliminary taxonomy of math search will be put forth, the major issues will be identified, methods for solving them will be discussed, and desirable future directions will be laid out. Achieving math-awareness in search, generation and use of math metadata, context-based math search, hit-relevance measures for math hits, interfacing, benchmarking and performance evaluation of math search systems, and portability of math search software across different math-content formats (LATEX, MathML, OMDOC, etc.), are some of the key aspects of math search that will be the focal points of discussion.

IC/MP218/012: Recent advances in software tools for scientific computing.

Organiser: Ronald Boisvert (National Institute of Standards & Technology, USA)
Co-organiser: Brian Ford (University of Oxford, UK)

Computation has become an indispensable tool for progress in science and engineering. For applied mathematicians and computer scientists who develop mathematical software tools, the central question remains the same as it was in the early days of computing: how should mathematical software be designed to get the highest performance possible, while remaining cost-effective to develop and maintain, as well as easy for users to deploy? The computing landscape today, however, is far different than it was when general purpose electronic computers emerged some 50 years ago. While processors have become cheap and ubiquitous, their underlying computer architectures have actually become more complex. Today such systems have multi-level hierarchical memory systems, multiple processors per chip, special-purpose co-processors, etc. On the Web, emerging service-oriented architectures (computational grids) envision the ad-hoc marshaling of disparate and widely distributed resources to attack computational problems and to share results. At the high end, hundreds to thousands of processors and memory systems are linked together into complex interconnection networks to address society's most challenging problems. Designers of mathematical software libraries, problem-solving environments, and related tools, which provide users with the capabilities needed to efficiently exploit such systems for practical use, are being challenged anew to develop scientific computing tools for this increasingly complex computing landscape. In this minisymposium, we will review how researchers and developers of scientific computing tools are addressing these issues. Speakers will review the state-of-the-art in mathematical software design, including emerging numerical algorithms, software architectures, user interfaces, testing methodologies, as well as some selected applications. (This minisymposium is dedicated to Dr. James C.T. Pool on the occasion of his recent retirement.)

Reflections on progress in software tools for numerical software. **Brian Ford** (University of Oxford, UK), Steve Hague (Numerical Algorithms Group (NAG), UK) IC/MT2403/012

We begin our reflections by considering the question: "What does the term *software tool* mean in the context of numerical software?" The short unhelpful answer to that question is "Different things to different people!". We will try to give a longer and more helpful answer by identifying various software tools which are indicative of the range of such tools, and which could be described as representing landmarks in the evolution of the discipline of numerical software engineering; that is ,the task of designing,developing,testing,documenting,porting and maintaining high quality software for numerically intensive applications. The field of numerical software has advanced significantly over the past forty years or so, and software technology has played a major part in that advance. We anticipate that the importance of such technology will continue in the future,not least in the area of software re-use, a practice long since embraced by the numerical software community but adopted only relatively recently by the world of computing generally. In numerical software terms,re-use means establishing desirable properties, such as robustness and accuracy, of a body of software, and then enabling the reliable and effective use of that software, with those properties intact, in different application or computational contexts. Since we cannot anticipate in all cases what those different contexts might be, this will always be "work in progress", but we will illustrate the progress made so far by referring to the NAG software development regime known as the Library Engine. This so called "engine" draws on numerous prior developments and experiments in software technology both by NAG itself and other numerical software practitioners, not least the pioneering work undertaken at Argonne National Laboratory in connection with the PACK projects, under the leadership of Jim Pool.

Mathematical software and Matlab. **Cleve Moler** (The MathWorks, Inc., USA) IC/MT1129/012

I will reminisce about the (not so recent) role of Jim Pool, Argonne, NAG, IMSL, WG2.5, Caltech, NASCAR, and the Tektronix 4081 in the development of LINPACK, EISPACK and MATLAB.

Recent progress in LAPACK and ScaLAPACK libraries for numerical linear algebra. **Sven Hammarling** (NAG Ltd, UK) IC/MT1569/012

In this talk we shall be looking at recent and forthcoming developments in the widely used LAPACK and ScaLAPACK numerical linear algebra libraries.

Improvements include the following: Faster algorithms with better numerical methods, memory hierarchy optimizations, parallelism, and automatic performance tuning to accommodate new architectures; more accurate algorithms, and the use of extra precision; expanded functionality, including updating and downdating and new eigenproblems; putting more of LAPACK into ScaLAPACK; and improved ease of use with friendlier interfaces in multiple languages.

After an overview, this talk will highlight new more accurate algorithms; faster algorithms, including those for pivoted Cholesky and updating of factorizations; and hybrid data formats. To accomplish these goals we are also relying on better software engineering techniques and contributions from collaborators at many institutions.

This is joint work with Jim Demmel, Jack Dongarra and the LAPACK/ScaLAPACK team.

The challenges of multicore and specialized accelerators for mathematical software. **Jack Dongarra** (Univ. Tennessee & Oak Ridge National Lab, USA) IC/MT1128/012

Recent versions of microprocessors exhibit performance characteristics for 32 bit floating point arithmetic (single precision) that is substantially higher than 64 bit floating point arithmetic (double precision). Examples include the IntelŠs Pentium IV and M processors, AMDŠs Opteron architectures, the IBMŠs Cell processor and various GPUs. When working in single precision, floating point operations can be performed up to two times faster on the Pentium and up to ten times faster on the Cell over double precision. The motivation for this work is to exploit single precision operations whenever possible and resort to double precision at critical stages while attempting to provide the full double precision results. The results described here are fairly general and can be applied to various problems in linear algebra such as solving large sparse systems, using direct or iterative methods and some eigenvalue problems. There are limitations to the success of this process, such as when the conditioning of the problem exceeds the reciprocal of the accuracy of the single precision computations. In that case the double precision algorithm should be used.

IC/MP218/012: Recent advances in software tools for scientific computing. #2

Organiser: Ronald Boisvert (National Institute of Standards & Technology, USA)
Co-organiser: Brian Ford (University of Oxford, UK)

(For abstract, see session #1 above.)

The evolution of software for computational optimization. **Jorge Moré** (Argonne National Laboratory, USA) IC/MT3500/012

We outline and discuss developments in computational optimization that have changed the way that large nonlinear optimization problems are formulated, analyzed, and solved. These developments include sophisticated algorithms and software, automatic differentiation tools, mathematical programming languages, and high-performance (parallel) architectures. The aim of these developments is to expand the range and size of optimization problems that can be modeled and solved by application scientists. We outline and discuss these developments in the context of our experiences with TAO (Toolkit for Advanced Optimization).

A test harness (TH) for high-performance numerical software. **Brian Smith** (University of New Mexico, USA) IC/MT1796/012

TH is a test harness to facilitate the development of scientific software. The operational model of the tool is the comparison of the results from two versions of an application code to ensure the results are equivalent. TH is first installed into an existing application code that runs to completion on a set of data. The application code with TH installed is run in generate mode to create a monitored data file. A second version of the application code with TH installed is run in check mode, comparing the current results with the original results, using criteria that tolerate expected rounding errors in the computation.

Features include specifiable criterion for data comparison,

process-independent check data formats, and a design that facilitates the installation of TH into codes written in any programming language and in parallel SPMD codes. Once installed, TH can be deactivated, permitting the same code to be maintained with and without the test harness in use.

A recent enhancement to TH is the implementation of a new set of tools installs TH into a Fortran application code with one of two default TH input files. One default file causes the test harness to monitor the execution sequence through specified procedures of the application and provide performance information for these procedures. The second default file specifies that the test harness monitors all Sexternal T variables of all selected procedures in the application at all entry points to and exit points from the specified procedures. An Sexternal T variable is defined to be any dummy argument, any variable accessed from a common block, or any variable accessed from a module. These default input files can be readily changed to specify the non-default comparison criteria.

Special functions, reference data and mathematical software. **Ronald Boisvert** (National Institute of Standards & Technology, USA) IC/MT1089/012

The Handbook of Mathematical Functions (Milton Abramowitz and Irene Stegun, eds.), a reference work published by the US National Bureau of Standards, remains the most cited work in the mathematical literature more than 40 years after its appearance in 1964. An important application of the Handbook has been in the development of tests for function evaluation software. NIST, in collaboration with some 40 external researchers, is developing the Digital Library of Mathematical Functions (DLMF), a new, Web-based handbook on the special functions of applied mathematics. Presenting such information in a way that is not only natural and convenient in a Web environment, but also provides capabilities that exceed what is available using traditional publication methods, remains a technical challenge. In this talk I will provide background on the DLMF project, with particular attention to the information technology issues related to the presentation of mathematics on the Web. A demonstration of DLMF facilities will be presented. Finally, applications to mathematical software development and testing will be described.

Evolution of mathematical software. **James Pool** (Prescott, Arizona, USA) IC/MT1625/012

The development and distribution of mathematical software has gone full circle in the last forty years. During the 1960s, mathematical routines were developed primarily by users and often contributed to collections accessible to other users. During the following two decades, a community of mathematical software developers emerged and focused on the creation of quality collections and libraries. However, during the past fifteen years, there has been a steadily increasing return to the approach of the 1960s. Why? We will review this evolution of the development and distribution of mathematical software, assess both the technical and non-technical causes of changing modes, and speculate on the future of mathematical software activities.

IC/MP311/012: High-level software for the numerical solution of partial differential equations.

Organiser: Robert Kirby (Texas Tech University, USA)
Co-organiser: Guido Kanschat (Texas A&M University, USA)
Co-organiser: Wolfgang Bangerth (Texas A&M University, USA)

The last decade has seen tremendous growth not only in raw computational power, but also in the sophistication of software for numerical computing. By providing high-level interfaces to powerful, mathematically robust methods such as finite elements, modern libraries greatly simplify and shorten the computational scientist's development cycle, improve productivity, and increase code reliability, frequently without a sacrifice of performance. All of these libraries to some extent provide support for structured or unstructured meshes, basis functions, and interfaces to powerful algebraic solvers. Some also include high-level support for variational forms, by which the algebraic systems are generated automatically from computational objects representing the variational problem. The speakers in this minisymposium will be the authors of several of these software libraries, and they will describe the design philosophy and capabilities of their codes. This minisymposium will allow developers of such codes to exchange ideas and potential users to gain a high-level introduction to emerging tools.

deal.II: a general-purpose object-oriented finite-element library. **Guido Kanschat** (Texas A&M University, USA), Wolfgang Bangerth (Texas A&M University, USA) IC/MT316/012

An overview of the software design and data abstraction decisions chosen for deal.II, a general-purpose finite element library written in C++, is given. The library uses advanced object-oriented and data encapsulation techniques to break finite element implementations into smaller blocks that can be arranged to fit users requirements. Through this approach, deal.II supports a large number of different applications covering a wide range of scientific areas, programming methodologies, and application-specific algorithms, without imposing a rigid framework into which they have to fit. A judicious use of programming techniques allows us to avoid the computational costs frequently associated with abstract object-oriented class libraries.

The paper presents a detailed description of the abstractions chosen for defining geometric information of meshes and the handling of degrees of freedom associated with finite element spaces, as well as of linear algebra, input/output capabilities and of interfaces to other software, such as visualization tools.

Parallel representation of topological data. **Dmitry Karpeev** (Argonne National Laboratory, USA) IC/MT1466/012

We have developed a flexible and scalable high-level framework for representation of topological data, such as, but not limited to, computational meshes, multigrid structures, high-degree graphs, networks, etc.

The novel feature of the approach is that the topological data, called Sieves, are treated with a minimal and flexible interface deriving in spirit from the formalism of cell complexes in combinatorial topology. Thus, the main relation of incidence is generalized in the spirit of Grothendieck to a single "covering" relation between entities in the Sieve. We identify the correct computational analog of such minimal topologies based on *operations* allowable Sieves, rather than attempting to mimic the formal mathematical structure. The minimal operations include 'closure', 'star', 'meet' and 'join', essentially in the same sense as for cell complexes but with a wider range of applicability, enabling navigation of the data.

While in traditional computational approaches the numerical data are inextricably linked to the topological data, we explicitly separate the two. Any Sieve can support *fields* - numerical data laid out over it regardless of the semantics (mesh coordi-

nates, physical fields etc). The ubiquitous domain decomposition approach is recognized as an instance of the *sheaf* property of fields, and implemented in a fashion appropriate for computational use. Specifically, we allow collections of Sieves (e.g., distributed among processors) to be related with an *overlap* Sieve. Fields can then be restricted to the overlap from individual Sieves as well as fused along the interface.

We will present the framework and illustrate its use in a range of scientific codes.

Automated solution of differential equations. **Anders Logg** (Simula Research Laboratory, Norway) IC/MT435/012

Differential equations are solved routinely by large computer programs, but the solution process is rarely automated. Each equation requires a different program and each such program requires a considerable amount of work to develop and maintain.

The FEniCS project provides a set of tools that automate important aspects of the solution process, ultimately aiming at a complete automation of computational mathematical modeling, including the automation of discretization, discrete solution, error control, modeling and optimization. A key component of FEniCS is the FEniCS Form Compiler (FFC), which automates the discretization of differential equations by taking as input a variational problem in mathematical notation and generating highly efficient optimized low-level code for the evaluation of the corresponding discrete operator.

In this talk, I will discuss key aspects and features of the FEniCS project and give a demonstration by specifying and solving a couple of standard differential equations.

Computing finite-element basis functions. **Robert Kirby** (Texas Tech University, USA) IC/MT1277/012

Access to general families of finite-element basis functions for H^1, $H(\mathrm{div})$, and $H(\mathrm{curl})$ of general order adds great value to the various high-level codes for meshes, solvers, and variational forms. I will talk about some recent developments for FIAT, the FInite element Automatic Tabulator. These include algebraically generating improved algorithms for evaluating functions at quadrature points.

IC/MP311/012: High-level software for the numerical solution of partial differential equations. #2

Organiser: Robert Kirby (Texas Tech University, USA)
Co-organiser: Guido Kanschat (Texas A&M University, USA)
Co-organiser: Wolfgang Bangerth (Texas A&M University, USA)

(For abstract, see session #1 above.)

GetDP: a general finite-element solver for the de Rham complex. **Christophe Geuzaine** (Université de Liège, Belgium) IC/MT1318/012

We present an overview of the structure of GetDP, an open-source software system started ten years ago with the goal of providing a high-level mathematical tool to solve partial differential equations using finite element-type techniques. The main feature of the software is the closeness between the organization of data defining a discrete problem (written by the user in an ASCII text file) and the symbolic mathematical expression of this problem. We show how the high-level decomposition of the problem into a limited number of objects makes the environment structured and concise, and permits the easy coupling of physical problems (electromagnetic, thermal, mechanical, etc.) and numerical methods, in various dimensions and time states.

This is joint work with Patrick Dular at the University of Liège.

FreeFem++, 2D finite-element PDE solver. **Frédéric Hecht** (Université Pierre et Marie Curie, France) IC/MT2143/012

Fruit of a long maturing process freefem, in its last avatar, FreeFem++, is a high-level integrated development environment (IDE) for numerically solvIng partial differential equations (PDE). It is the good tool for teaching the finite element method but it is also perfect for research to quickly test new ideas or multi-physics and complex applications.

A partial differential equation is a relation between a function of several variables and its (partial) derivatives. Many problems in physics, engineering, mathematics and even banking are modeled by one or several partial differential equations.

FreeFem++ is a software to solve these equations numerically. It is not a package, it is an integrated product with its own high level programming language . This software runs on unix, Windows and MacOS X.

Moreover FreeFem++ is highly adaptive. Many phenomena involve several coupled system, for example: fluid-structure interactions and ocean-atmosphere problems are such systems. These require different finite element approximations degrees, possibly on different meshes. Some algorithms require data interpolation on multiple meshes within one program.FreeFem++ can handle these difficulties, i.e. *arbitrary finite element spaces on arbitrary bidimensional meshes*.

FreeFem++ has an advanced automatic mesh generator, capable of *a posteriori* mesh adaptation; it has a general purpose elliptic solver interfaced with fast algorithms such as the multi-frontal method UMFPACK. Hyperbolic and parabolic problems are solved by iterative algorithms prescribed by the user with the high level language of FreeFem++. It has several triangular finite elements, including discontinuous elements. Finally everything is there in FreeFem++ to prepare research quality reports: color display online with zooming and other features and postscript printouts.

The web site is http://www.freefem.org/ff++

A modern and unified C++ implementation of finite-element and spectral-elements methods in 1D, 2D and 3D: overview and applications. **Christophe Prudhomme** (Université Grenoble I, France) IC/MT3504/012

We present in this talk a modern and unified C++ implementation of finite and spectral element methods in 1, 2 and 3D that provides a mathematical kernel for a number of complex multiphysics and multiscale simulations, such as fluid structure interaction or mass transport, in the context of haemodynamics. The main result consists of a library of components that provides domain-specific abstractions, in our case numerical analysis tools, using generic, meta-programming and object-oriented paradigms. At the top of these components sits a so-called domain-specific language embedded in C++ that allows to formulate variational problems in terms close to the mathematics. This has a number of advantages among which high-level expressivity and using implicitly the properties of the C++ compilers such as their optimization framework and their programming environments — preprocessor, libraries... — We shall demonstrate this kernel through applications in blood flow and multi-fluid flow simulations.

IC/MP125/012: Image processing: computation and applications.

Organiser: Choi-Hong Lai (University of Greenwich, UK)
Co-organiser: Meiqing Wang (Fuzhou University, PR China)

There are many applications of image processing in industry and also for personal leisure. Examples include media applications, video on demand, archive management, digital library, underground-piping recognition/examination, crack location, groundwater flow, soil properties, image restoration for historical heritage, image de-blur, image impainting, etc. Many of these examples require fast computer hardware and good numerical methods to reach industrial standards. Researchers from the major fields of mathematics and computer science are required to collaborate in order to achieve the best results. This mini-symposium provides a forum for scientists and practitioners, in the main areas of mathematics, computer science, and image processing to exploit and enhance techniques for image processing making them viable for industrial applications. The theme of the mini-symposium concerns all aspects of image processing, including image compression, image de-noising, image restoration, parallel processing, and their industrial applications. Use of partial differential equations will be examined for image de-noising, image de-blur, and image impainting. Use of fractals and wavelets for image compression and de-compression will be examined for video and archive applications. State-of-the-art parallel algorithms for image processing are also included in the dissemination.

Video compression using fractal and color-transfer algorithm. **Meiqing Wang** (Fuzhou University, PR China), Sihui Chen (Fuzhou University, PR China), Choi-Hong Lai (University of Greenwich, UK) IC/MT480/012

Recently many methods for achieving high compression ratios in video compression have appeared in literature and in the industry, including MPEG, H.263, JPEG, wavelets and fractals. Among these methods, the fractal method is a feasible and promising compression technique due to its low complexity in the process of decompression and high compression ratio. Handling colour images using fractals is important in the digital images and human visual system because colour images are almost indispensable for human perception. In the study of color images, color transfer algorithms are usually used to convert an image's colors which lead the conversion of the image's scene. In this paper we use color transfer technology in fractal video compression to obtain a high compression ratio. As used in other fractal methods, a given sequence of images is divided into groups of frames (about four or five frames in a group). The first frame of each group is compressed by an efficient fractal color image compression method. The remaining frames of the group are converted into gray images, which are then compressed using the adaptive fractal gray image compression method. During the process of decompression, the first frame is decompressed using the corresponding decompression method. For the remaining frames of the group, the corresponding fractal gray video decompression method is used to obtain the gray image sequence, and the sequence is then converted to color ones using the color transfer algorithm by passing the colors of the first frame to the remaining ones of the group. In the experiments two different color transfer algorithms are applied to some video frames. Experimental results show that the algorithm not only is able to obtain a high reconstruction quality (the PSNR value of the decompression video images are about 30), but also can achieve a high compression ratio (above 30) without perceptible image degradation.

Exploiting statistical properties of wavelet coefficient for face detection and recognition. **Naseer Aljawad** (The University of Bukingham) IC/MT495/012

Wavelet transforms (WT) are increasingly becoming an essential tool for image processing and analysis. Image and video compression, image watermarking, content-base image retrieval, face recognition, texture analysis, and image feature extraction are all but few examples. The Wavelet Transform is a technique for analyzing finite-energy signals at multi-resolutions. It provides an alternative tool for short time analysis of quasi-stationary signals, such as speech and image signals, in contrast to the traditional short-time Fourier transform. The Discrete Wavelet Transform (DWT) is a special case of the WT that provides a compact representation of a signal in the time and frequency domain. In particular, wavelet transforms are capable of representing smooth patterns as well anomalies (e.g., edges and sharp corners) in images. In this presentation, we are focusing using wavelet transforms for facial feature detection.

There are a number of different wavelet image-decomposition schemes. The most commonly used scheme is the pyramid scheme, which we have adopted. At a resolution depth of k, the pyramidal scheme decomposes an image I into $3k+1$ frequency subbands $(\mathrm{LL}_k, \mathrm{HL}_k, \mathrm{LH}_k, \mathrm{HH}_k, ..., \mathrm{HL}_1, \mathrm{LH}_1, \mathrm{HH}_1)$. the lowest-pass subband LL_k representing the k-level resolution approximation of the image I, while the other high-frequency sub-bands highlight the significant image features at different scales. Interestingly, the histogram of the LL sub-band is an approximation of that of the original image, while the coefficients in each of the other subbands have a Laplacian (also called generalised-Gaussian) distribution. In this presentation we shall review various techniques that exploit the statistical properties and parameters of the non-LL sub-bands to locate and detect faces in images/videos. We shall present test results to measure the performance of these techniques using bench-marked audio-visual images/video.

MPEG-4 video transmission over UMTS mobile networks. **Maaruf Ali** (Oxford Brookes University, UK) IC/MT679/012

This talk will present an overview of MPEG-4, covering the structure of MPEG-4 coded video files and the VOP types. Followed by classification of errors and introduction of the NEWPRED mechanism in MPEG-4 for error concealment. An UEP (Unequal Error Protection) scheme will also be described ending with how the application of the proposed scheme is used in quanitifying improvements in the UMTS network efficiency.

Application of the topological gradient to image processing. **Mohamed Masmoudi** (Université Paul Sabatier Toulouse III, France) IC/MT947/012

The goal of most image processing problems is to split the image in several parts. This is the case of classification, segmentation and edge detection problems.

To find a part of an image is equivalent to find its characteristic function. At first sight this problem is not differentiable, but using calculus of variation methods, it is possible to derive the variation of a cost function when we switch the characteristic function from 0 to 1 or from 1 to 0 in a small area. This variation is called the topological gradient.

This gradient type information allows to build very fast algorithms. In most applications the solution is obtained in only one iteration.

We first recall the basic concept of topological gradient and its applications to optimal design and imaging. Then we con-

sider some image processing problems under the topological gradient point of view.

We present its application to edge detection, by inserting small cracks in the image. The restoration of noisy images is then pretty straightforward. Some restorations of short video sequences will be presented.

To restore hidden parts of an image (inpainting), the edges (or cracks) of the known image are propagated inside the hidden part. The restoration is done using diffusive approaches taking into account the insulating edges.

IC/MP125/012: Image processing: computation and applications. #2

Organiser: Choi-Hong Lai (University of Greenwich, UK)
Co-organiser: Meiqing Wang (Fuzhou University, PR China)

(For abstract, see session #1 above.)

Two-phase methods for deblurring images corrupted by impulse plus Gaussian noise. **Raymond Chan** (Chinese University of Hong Kong) IC/MT140/012

We consider the problem of restoring blurred images which are corrupted by impulse noise and possibly Gaussian noise. We solve the problem in two phases. In the first phase, median-type filters are applied to locate the pixels which are likely to be corrupted by impulse noise. In the second phase, we solve an inverse problem from incomplete data by a variational method. More precisely, we minimize a regularized functional involving only the data samples detected as outlier-free in the first phase. The experiments show that our method is 4–7 dB better in PSNR than a full variational methods for image deblurring under impulse noise. Moreover, our scheme can restore blurred images corrupted by 90% salt-and-pepper noise or 50% random-valued impulse noise.

Parallel computing algorithms and CAGD processing methods for fractal images in virtual geographic environments. **Dan Liu** (Dalian Maritime University, PR China) IC/MT154/012

This talk starts with the theory and applications of Nonlinear Mathematics, develops the research on basic theory and methods of geographic Fractal model computing in virtual geographic environment with very strong applying background, establishes scientific parallel computing model, designs more effective parallel computing algorithm of geographic Fractal models. After exploiting and founding common parallel landscape simulation theory, combines the related techniques and methods of Fractal, Wavelet and CAGD(Computer Aided Geometric Design), constructs high dimensional Fractal algorithm, synchronic Fractal display algorithm of 3D multi-channel scene, texeture synthesizing algorithm based on shape surfaces etc. As we all known, the Fractal simulation technique can achieve high fidelity when it is used to simulate nature scenery, the main drawback of such techniques is the very high computing time needed to determine the realtime display;in addition, the key actual physiognomy simulation technique CAGD is not very good at dealig with 3D nature anomalistic objects. The talk will also introduce some research on parallel computing of geographic Fractal models, including correlative system configuration, parallel algorithm and parallel programme, the shown results have improved the fidelity of mutual simulation system and the generating speed of Fractal images greatly, produced complicated 3D physiognomy simulation with arbitrary distinguished degree, and altered the states of the simulated entities dynamically.

Bilinear interpolation for image conversion between square structure and hexagonal structure. **Xiangjian He** (University of Technology, Sydney, Australia) IC/MT387/012

Spiral Architecture (SA) is a relatively new and powerful approach to machine vision system. The geometrical arrangement of pixels on SA can be described as a collection of hexagonal pixels. However, all the existing hardware for capturing image and for displaying image are produced based on rectangular architecture. Therefore, it becomes important to find a proper software approach to mimic SA so that images represented on the traditional square structure can be smoothly converted from or to the images on SA. For accurate image processing, it is critical to best maintain the image resolution during the image conversion. In this paper, we present an algorithm for bilinear interpolation of pixel values for image conversion between square structure and the simulated SA. The comparison in terms of representation accuracy is performed and demonstrated using experimental results.

Gradient-field computation and its application in image inpainting. **Choi-Hong Lai** (University of Greenwich, UK), Meiqing Wang (Fuzhou University, PR China), Xunxun Zeng (Fuzhou University, PR China) IC/MT462/012

The task of filling in missing or damaged regions of an image is known as image inpainting which has many important applications in the area of digital image processing. The BSCB model proposed by Bertalmio et al., pioneered a digital image inpainting algorithm based on partial differential equations (PDEs). The basic idea is to smoothly propagate information from the surrounding areas in the isophote directions. A new method for computing the gradient field combined with a max/min function is proposed as the information propagating estimator to improve the BSCB model. Since the above improved method provides good results at corners, it is also applied to the Euler's elastica model. Numerical experiments show that the modified methods can repair the images well, especially along edges and at corners.

IC/MP86/012: Writing scientific software: experience with using, developing and teaching.

Organiser: Osni Marques (Lawrence Berkeley National Laboratory, USA)
Co-organiser: Suely Oliveira (The University of Iowa, USA)

Writing scientific software requires attention to both numerical and software engineering aspects. Performance trade-offs in using modern programming languages and systems can be difficult to understand, but are crucial for many applications. While the basic development of new ideas can be implemented using basic interactive tools, at the high-performance edge, software has to be carefully designed, documented, and tuned for future updates.

In this minisymposium we bring together speakers from National Labs and academia who work with numerical and software aspects of scientific programming. We will emphasize experience in using, developing and teaching scientific software.

Scientific programming as a science. **Paolo Bientinesi** (Duke University, USA), Robert van de Geijn (University of Texas at Austin, USA), Enrique Quintana-Orti (Universitat Jaume I, Spain) IC/MT249/012

In recent years it has become customary to use clusters of hundreds of computers for running large scientific computations. The programming paradigm was that of distributed memory parallel systems. With the advent of SMP and multi-core systems, we are now moving towards hybrid platforms in which distributed memory and shared memory paradigms live together. Multi-core systems with dozens of cores may become the norm within a decade. Writing and tuning high-performance software in such environments is challenging. Besides, in order to attain maximum performance, additional algorithms, with respect to the ones commonly used in a sequential environment, will have to be developed. This further increases the burden on the programmers.

In this talk we show how a high-level notation and a goal-oriented approach can be used to systematically develop high-performance linear algebra libraries. These libraries contain several algorithms for each target operation and can be created in a number of target languages. The methodology, developed as part of the FLAME project at UT-Austin, is powerful enough to create libraries like LAPACK, yet simple enough that it can, and has been, taught at the undergraduate level. The key is to approach high-performance programming with rigorous tools from computer science as opposed to ad-hoc methods.

Life as a developer of numerical software. **Sven Hammarling** (NAG Ltd, UK) IC/MT251/012

Rewards of readily-available software tools. **Leroy Anthony Drummond-Lewis** (Lawrence Berkeley National Laboratory, USA), Osni Marques (Lawrence Berkeley National Laboratory, USA) IC/MT1756/012

The US Department of EnergyŠs (DOE) Advanced Computational Software (ACTS) Collection comprises a set of software tools that make it easier for application developers to write high performance codes for high-end computers. The development of such codes is often a demanding process, due to the complexity of the phenomena to be simulated but also to the proliferation and evolution of computer architectures. ACTS tools have lessened the development effort in a number of cases, and also contributed for an optimal usage of the available, and often scarce, computational resources. The tools fall into four broad categories: implementation of numerical algorithms, frameworks, execution support and developer support. This presentation will focus on the functionalities currently available in the collection; lessons that have been learned through an interaction with tool developers and; the rewards of outreach efforts and hands-on activities; and scientific applications that have benefited from the tools.

Scientific programming and object-oriented approaches, with emphasis on multigrid software. **Ricardo Ortiz** (University of Iowa, USA), Suely Oliveira (The University of Iowa, USA) IC/MT1975/012

Many problems in scientific computing require a large amount of computations. The reason for this may be because the problem requires or produces large amounts of data or simply because of the problem's complex nature. For this reason we need to write scientific code that is easy to read, reusable and at the same time performs computations accurately and efficiently. Ever since the 1950s, the complexity of scientific software has been increasing. Object oriented techniques have been developed to alleviate this complexity and now more people are writing scientific software in C and C++ like languages. We present a multilevel algorithm framework written in C++ for solving large scale linear system of equations and discuss some of the programming techniques used to improve code readability and achieve peak performance. The design of the framework is separated into a series of modules that allow us to debug the code faster and test its performance in an easy and systematic way.

IC/MP221/012: Combinatorial scientific computing.

Organiser: Alex Pothen (Old Dominion University, USA)

Combinatorial scientific computing (CSC) is an interdisciplinary research area in which combinatorial mathematics and algorithms are employed to solve problems in scientific computing. While research in CSC has been ongoing since the 1970's, the CSC research community has been fragmented because the myriad roles of combinatorial methods are scattered in standard taxonomies of scientific computing. In order to address this fragmentation, the CSC community has organized three international workshops since 2004, two of them sponsored by SIAM. This minisymposium affords an opportunity for members of the CSC community to interact with the global applied mathematics community.

The eight speakers in this minisymposium will discuss recent research on a collection of CSC topics. Among these are: graph matching models and algorithms for computing good orderings for factoring sparse matrices; support theory methods for computing novel, combinatorial preconditioners for solving sparse linear systems of equations; hypergraph partitioning for load-balancing in parallel computing; combinatorial problems in automatic differentiation; specialized graph coloring problems and coloring algorithms to efficiently compute large-scale Jacobians and Hessians; practical parallel algorithms for combinatorial problems on massively parallel computers, etc.

Developments in matching and scaling algorithms. **Iain Duff** (Rutherford Laboratory & CERFACS, UK) IC/MT3235/012

For many years the HSL code MC64 developed by Duff and Koster (SIMAX 22 pp.973–996) has been used primarily as a preprocessing step for both iterative and direct solvers. We discuss enhancements to this code and, in particular, examine its use in predetermining pivot sequences for symmetric indefinite factorization. We demonstrate its use as an analysis tool with the HSL symmetric indefinite code MA57. This work is based on joint work with Stephane Pralet, Samtec, Liege, Belgium. We also illustrate how a similar approach can be used in a code for the direct solution of sparse skew symmetric matrices.

An option in MC64 provides a scaling so that the scaled system can be permuted so that the diagonal has value one and all off-diagonal entries are less than or equal to one in modulus. We compare the effect of using this scaling compared with a scaling that tries to make all entries close to one and another that makes the scaled matrix doubly stochastic. We compare these approaches both in the context of direct and iterative solvers.

Matching algorithms in scientific computing. **Florin Dobrian** (Old Dominion University, USA), Mahantesh Halappanavar (Old Dominion University, USA), Alex Pothen (Old Dominion University, USA) IC/MT2933/012

We discuss the combinatorial optimization problem of graph matching in the context of scientific computing. Matching has a special place among combinatorial optimization problems because, although not ubiquitous, it can be solved optimally in polynomial time. Therefore, from a theoretical perspective, matching algorithms are considered to be efficient.

In practice, however, polynomial time complexity is not necessarily equivalent to efficiency. The time complexity of matching algorithms is actually superlinear and it may take too long to compute a matching in a very large graph. In order to address this issue one can attempt either to employ fast approximation algorithms, which compute suboptimal solutions, or to rely on parallelization. However, exact matching algorithms, i.e., matching algorithms that compute optimal solutions, tend to be difficult to parallelize and parallelization may have to rely on approximation as well in high performance matching codes.

One area with a strong emphasis on high performance is scientific computing, where advanced scientific problems are simulated on highly sophisticated supercomputers. Graph matching can be used in scientific computing as a technique for modeling various sparse matrix computations, which represent basic scientific computing tools. In this talk we present new efficient modeling techniques for sparse matrix computations that are based on graph matching algorithms, the algorithms employed being both exact and approximation. Through theoretical and experimental results we show that the new techniques can outperform those that were previously used in modeling sparse matrix computations.

Hierarchical coloring. **Paul Hovland** (Argonne National Laboratory, USA) IC/MT4198/012

Discretizing PDEs on a regular grid induces a hierarchy of two types of sparsity patterns on a Jacobian matrix, one due to the stencil being used and one due to the dependence among individual degrees of freedom within that stencil. Goldfarb and Toint demonstrated how to exploit the sparsity structure induced by the stencil, but exploiting the unstructured sparsity within the stencil must rely upon more general techniques. We present a two stage coloring strategy: Goldfarb-Toint coloring followed by optimal intra-stencil coloring. We demonstrate that optimal coloring at both stages is suboptimal in general. Nonetheless, savings of 50% or more over Goldfarb-Toint alone are possible.

Computing Hessians without tears: automatic differentiation and graph coloring. **Alex Pothen** (Old Dominion University, USA) IC/MT4153/012

Interior-point methods for nonlinear optimization problems require second-order derivatives of the Lagrangian function, and exact Hessians are needed in parametric sensitivity analysis. A sparse Hessian matrix can be computed accurately using automatic differentiation via a three-step procedure. First, using the nonzero pattern of a Hessian, we partition its columns into groups, such that the nonzeros in the columns of a group can be computed together. Second, we compute the numerical values of the nonzeros in each group of columns in the partition by automatic differentiation. Finally, we recover the values of the nonzeros in the Hessian from the values in the groups in the partition. The first step is accomplished by a specialized graph coloring: a star coloring, if the nonzero values in the Hessian are computed by solving a diagonal system of equations; or an acyclic coloring, if the nonzeros are computed by solving a triangular system of equations. We describe new algorithms for the first and third steps, and integrate our codes with ADOL-C, a software tool for automatic differentiation. Our results show that evaluating a Hessian via a triangular substitution method using acyclic coloring is currently the fastest method, and that this approach makes the computation of Hessians with hundreds of thousands of columns feasible.

IC/MP221/012: Combinatorial scientific computing. #2

Organiser: Alex Pothen (Old Dominion University, USA)

(For abstract, see session #1 above.)

Combinatorial preconditioners for scalar elliptic finite-element problems. **Haim Avron** (Tel Aviv University, Israel), Gil Shklarski (Tel Aviv University, Israel), Sivan Toledo (Tel Aviv University, Israel) IC/MT2852/012

We present a new preconditioner for linear systems arising from finite-elements discretizations of scalar elliptic partial differential equations (PDE's). The linear system is denoted $Kx = b$, where K is the global stiffness matrix and is a sum $K = \sum_e K_e$ of element matrices. The solver splits the collection $\{K_e\}$ of element matrices into a subset $E(t)$ of matrices that are approximable by diagonally-dominant matrices and a subset of matrices that are not approximable. The approximable K_e's are approximated by diagonally-dominant matrices L_e's that are scaled and assembled to form a global diagonally-dominant matrix $L = \sum_{e \in E(t)} \alpha_e L_e$. A combinatorial graph algorithm approximates L by another diagonally-dominant matrix M that is easier to factor. The inapproximable elements are added to M and the sum $M + \sum_{e \notin E(t)} K_e$ is factored and used as a preconditioner. When all the element matrices are approximable, which is often the case, the preconditioner is provably efficient. Experimental results show that on some problems, the preconditioner is more effective than an algebraic multigrid solver, than an incomplete-factorization preconditioner, and than a direct solver.

Hypergraphs in scientific computing. **Rob Bisseling** (Universiteit Utrecht, The Netherlands) IC/MT2391/012

In the past decade, hypergraphs have emerged as a powerful tool in scientific computing applications. Hypergraph partitioning is the method of choice for distributing the data for sparse matrix–vector multiplication in an iterative linear system solver, or in a parallel computation of the PageRank eigenvector, which represents the ranking of web pages. Hypergraph clustering can be used to find related documents in large text collections, or in biological data sets.

This talk gives a survey of current and potential hypergraph applications, and discusses the use of the Mondriaan matrix partitioning package as a more general hypergraph tool. Furthermore, it presents recently added features such as scaled inner product matching, hybrid Mondriaan–fine grain partitioning, and a MATLAB interface.

Combinatorial models and algorithms for parallel sparse matrix distributions. **Erik Boman** (Sandia National Laboratories, USA) IC/MT2566/012

Sparse matrix-vector multiplication is an important kernel in scientific computing. This is the core of iterative linear solvers. For parallel computing, reducing the communication is crucial. This is a rich combinatorial problem. We first review classic graph and hypergraph models for sparse matrix partitioning, and then present new models for 2d fine-grain matrix partitioning. We discuss graph algorithms for our new approach. Preliminary results will be presented.

Hypergraph-based dynamic load-balancing for adaptive scientific computations. **Ümit Çatalyürek** (The Ohio State University, USA), Karen Devine (Sandia National Laboratories, USA), Erik Boman (Sandia National Laboratories, USA), Doruk Bozdağ (The Ohio State University, USA) IC/MT2585/012

Load-balancing (also known as *partitioning*) is a critical component in parallel scientific computing to achieve higher degree of parallelism. The goal is to assign computation to processors evenly while trying to minimize the communication volume. This assignment occurs at the start of a computation (*static* partitioning), but often, reassignment of work is done during a computation (*dynamic* partitioning) as the work distribution changes over the course of a computation. Hypergraph-based load balancing has proved to be successful for static load balancing problem in scientific computations, and partitioning software for the static case is widely available. In this talk, we present a new hypergraph model for the dynamic case, where we minimize the sum of communication in the application plus the migration cost to move data, thereby reducing total execution time. The new model can be solved using hypergraph partitioning with fixed vertices. We describe an implementation of a parallel multilevel partitioning algorithm within the Zoltan load-balancing toolkit, which to our knowledge is the first code for dynamic load balancing based on hypergraph partitioning. Finally, we present experimental results that demonstrate the effectiveness of our approach.

IC/MP172/014: The role of scale and orientation in mathematical image analysis.

Organiser: Arjan Kuijper (RICAM Linz, Austria)

Image analysis is concerned with analyzing the contents of images without *a priori* knowing them. Methods performing this task are usually validated by human observers. Challenging tasks are therefore to define mathematical models that mimic the human brain, and to understand them. The latter requires knowledge of various mathematical fields, like topology, geometry, PDEs, singularity theory, and statistics.

In this mini-symposium requirements for such methods, like scale and orientation of objects are discussed. The mathematical properties of these so-called *scale-space* methods are exploited. This results in models that capture essential characteristics of images. They allow, for instance, a simpler representation, enhancing, and reconstruction of an image. The speakers in this mini-symposium have a strong background in image analysis based on scale-space methods. They will present the current state-of-the-art for these approaches.

Image analysis using p-Laplacian and geometrical PDEs. **Arjan Kuijper** (RICAM Linz, Austria) IC/MT767/013

Minimizing the integral $\int_\Omega |\nabla u|^p \mathrm{d}\Omega$ for an image u under suitable boundary conditions gives PDEs that are well-known for $p = 1, 2$, namely Total Variation evolution and Laplacian diffusion (also known as Gaussian scale space and heat equation), respectively. Without fixing p, one obtains a framework related to the p-Laplace equation. The partial differential equation describing the evolution can be simplified using gauge coordinates (directional derivatives), yielding an expression in the two second order gauge derivatives and the norm of the gradient. Ignoring the latter, one obtains a series of PDEs that form a weighted average of the second order derivatives, with Mean Curvature Motion as a specific case.

Both methods have the Gaussian scale space in common. Using singularity theory, one can use properties of the heat equation (namely. the role of scale) in the full (Ω, t) space and obtain a framework for topological image segmentation.

The general frameworks will be presented and its properties discussed. The relations with gauge coordinate descriptions of the PDEs are shown, as well as filtering properties of solutions of some of these PDEs. Also examples of its use in image evolution and analysis will be given. Relations with the other talks in this mini-symposium will be pointed out.

Coarse-to-fine partitioning of signals. **Luc Florack** (Technische Universiteit Eindhoven, The Netherlands) IC/MT1440/013

We introduce the multiscale extension of a positive, real-valued signal $f(x)$,

$$u(x,s) = \exp\left(s\, d^2/dx^2\right) f(x)\,,$$

and the auxiliary signal

$$g(x,s) = \frac{1}{2}\, u_x^2(x,s)\,.$$

We write $u_0^{(k)}$ for a k-th order x-derivative at $(x,s)=(0,0)$, and assume $u_0^{(k)} \neq 0$ unless stated otherwise. We consider two partitioning methods, based on the spatial critical paths defined by $u_x(x,s)=0$, respectively $g_x(x,s)=0$.

(i) $u_x(x,s)=0$:

- $u_0^{(1)}=0$ corresponds to a regular critical path.
- $u_0^{(1)}=u_0^{(2)}=0$ indicates an annihilation event. In Thom's "List of the Seven Elementary Catastrophes" this represents a fold catastrophy, with control parameter s.
- Inflection paths defined by $u_{xx}(x,s)=0$ provide separatrices in (x,s)-space, separating peaks, dales, and void regions. They connect in a similar annihilation event.

(ii) $g_x(x,s)=0$:

Type I: $u_x(x,s)=0$:

- $u_0^{(1)}=0$ corresponds to a regular critical path.
- $u_0^{(1)}=u_0^{(2)}=0$ corresponds to a "pitchfork": 3 regular critical paths for $s<0$ meet at the origin, leaving 1 for $s>0$. In Thom's list this represents a fold catastrophy, with 1 control parameter, viz. s.

Type II: $u_{xx}(x,s)=0$:

- $u_0^{(2)}=0$ corresponds to a regular critical path.
- $u_0^{(2)}=u_0^{(3)}=0$ indicates an annihilation event. (No critical points of u are involved.) In Thom's list this represents a cusp catastrophy with 2 control parameters, s and $u_0^{(1)}$.

Upon increasing scale all regions, including void, will merge into an encompassing region. Under mild conditions there exists a scale $S>0$ such that there is only one extremum for $s>S$, viz. a maximum. In this way we obtain a coarse-to-fine partitioning of the signal.

(The Netherlands Organisation for Scientific Research (NWO) is gratefully acknowledged for financial support.)

Multi-scale singularity trees. **Jon Sporring** (Københavns Universitet, Denmark) IC/MT2525/013

We propose and experimentally evaluate a novel scale-space image hierarchies called Multi-Scale Singularity Trees (MSSTs). For an n dimensional image, the spatial critical points ar extended to 1-dimensional manifolds (curves) in the $n+1$ dimensional space space - the image and its Gaussian blurred versions at all scales. These curves contain catastrophe points, where spatial saddle and extrema parts are joined.

MSSTs are constructed by connecting annihilating catastrophe

points based on the nesting of image segments in the scale-space. Because of the only generic catastrophes are the pairwise interactions between critical points in scale-space and two catastrophes never occur at the same scale, MSSTs are always rooted ordered binary tree.

MSSTs are powerful and unique because of their simple binary structure and straightforward construction method, and most importantly, their soft-linked nature, where all connections in MSSTs are accompanied by their strengths. Using the matching algorithm developed specifically for MSSTs to fully exploit their unique properties, the usefulness and performance of MSSTs are further shown experimentally.

Cahn–Hilliard inpainting and the Willmore functional. **Carola-Bibiane Schönlieb** (Universität Wien, Austria), Martin Burger (Universität Münster, Germany) IC/MT1234/013

The Cahn-Hilliard equation has its origin in material sciences and serves as a model for phase separation and phase coarsening in binary alloys. A new approach in the class of fourth order inpainting algorithms is inpainting of binary images using the Cahn-Hilliard equation proposed in [1]. Like solutions of the Cahn-Hilliard equation converging to two main values during the phase separation process, the grayvalues inside the missing part of the image are oriented towards the binary states black and white. My talk in this minisymposium is devided in two main parts. First I will present stability/instability results for solutions of the Cahn-Hilliard equation and their connection to the Willmore functional, mainly presented in [2]. In particular we will consider the Willmore functional as a quantity to find the optimal scale of the inpainting result. Further I will give some analytic results for the modified Cahn-Hilliard equation. In a subsequent work of [1] the authors present a first analysis including also existence and regularity results. We will extend these considerations with results for the stationary state and a special discretization.

References:

[1] Bertozzi, A., Esedoglu, S., Gillette, A., Inpainting of binary images using the Cahn-Hilliard equation, to appear in IEEE Trans. Image Proc., 1-6.
[2] Burger, M., Chu, S.-Y., Markowich, P., Schönlieb, C., The Willmore functional and instabilities in Cahn-Hilliard. In preparation, 1-19.

IC/MP172/014: The role of scale and orientation in mathematical image analysis. #2

Organiser: Arjan Kuijper (RICAM Linz, Austria)

(For abstract, see session #1 above.)

Scale-space salient points. **Marco Loog** (Københavns Universitet, Denmark) IC/MT1983/013

We investigate statistical approaches to detect salient points in images; i.e., those locations that stand out conspicuously. The first one takes on a discriminatory standpoint, while the second one investigates the problem based on information theoretical considerations. Generally, both these approaches rely, either explicitly or implicitly, on a Bayesian rationale.

- In the discriminatory setting, classification tools from statistical pattern recognition and machine learning are employed. The basic underlying theory is that salient points are those that are easily discernable in the image; that is, they are readily discriminated from their surroundings. As we will show, discernibility can be quantified in terms of a supervised classification task and, consequently, it provides the statistical means to quantify this notion. As a result of this, learning tools can be utilized in the search for interest points.
- A different way of quantifying saliency is by means of the amount of information that a point adds to its surroundings. Informative points represent something of interest in an image scene and they can therefore be considered the salient points sought after. In this approach, the relative entropy, or the Kullback-Leibler divergence, will be the measure of prime interest that will be employed to provide a statistical information-driven quantity that describes the degree of saliency.

The fact that [physical] measurements should take place by means of apertures of finite size, also has its effect on how the salient point detection is actually carried out. In principle, point estimations cannot be performed and the information needed in both of the foregoing methods, typically has to come from neighborhood operators as provided by a Gaussian scale space framework. Consequences regarding information representation and saliency detection will also be discussed.

MR image reconstruction using the iterative-refinement method and nonlinear inverse scale-space methods. **Lin He** (RICAM Linz, Austria) IC/MT5016/013

Magnetic resonance imaging (MRI) reconstruction from sparsely sampled data has been a difficult problem in medical imaging field. We approach this problem by formulating a cost functional that includes a constraint term that is imposed by the raw measurement data in k-space and the L1 norm of a sparse representation of the reconstructed image. The sparse representation is usually realized by total variational regularization and/or wavelet transform. We have applied the Bregman iteration to minimize this functional to recover finer scales in our recent work. Here we propose nonlinear inverse scale space methods in addition to the iterative refinement procedure. Numerical results from the two methods are presented and it shows that the nonlinear inverse scale space method is a more efficient algorithm than the iterated refinement method.

Contour enhancement and completion via left-invariant second-order stochastic evolution equations on the 2D Euclidean-motion group. **Remco Duits** (Technische Universiteit Eindhoven, The Netherlands) IC/MT2518/013

Given an image $f : \mathbb{R}^2 \to \mathbb{R}$ we construct a local orientation score $U_f : SE(2) \to \mathbb{C}$, which is a complex-valued function of the Euclidean motion group $SE(2)$. The transformation $f \mapsto U_f$ is a wavelet transform constructed by an oriented wavelet $\psi : \mathbb{R}^2 \to \mathbb{C}$ and a representation $\mathcal{U} : SE(2) \to \mathcal{B}(\mathbb{L}_2(\mathbb{R}^2))$ of $SE(2)$, which boils down to convolutions with the oriented wavelet rotated at multiple angles. Under conditions on ψ the wavelet transform is unitary, inducing well-posed image reconstruction by the adjoint. This allows us to relate operators on images to operators on orientation scores in a robust way. To obtain Euclidean invariant image processing the operator on the orientation score must be left invariant. Therefore we consider left-invariant scale spaces on the Euclidean motion group $SE(2)$ generated by a quadratic form on left invariant vector fields of $SE(2)$. These scale spaces correspond to well-known stochastic processes on $SE(2)$ for contour completion and contour enhancement. The linear scale spaces on $SE(2)$ are given by group convolution with the corresponding Green's functions which were hitherto unknown. We derive the *exact* Green's functions and suitable approximations on a Group of

Heisenberg type, which we use together with the framework of invertible orientation scores for automatic contour enhancement and completion. We also consider *non-linear, adaptive* scale spaces on $SE(2)$ and their practical value in coherent enhancing diffusion.

Coordinate-free diffusion over compact Lie-groups. **Yaniv Gur** (Tel Aviv University, Israel), Nir Sochen (Tel Aviv University, Israel) IC/MT1421/013

We have seen in recent years a need for regularization of complicated feature spaces: Vector fields, orientation fields, color perceptual spaces, the structure tensor and Diffusion Weighted Images (DWI) are few examples. In most cases we represent the feature space as a manifold. In the proposed formalism, the image is described as a section of a fibre bundle where the image manifold is the base space and the feature space is the fibre. In some distinguished cases the feature space has algebraic structure as well. In the proposed framework we treat fibres which are compact Lie-group manifolds (e.g., $O(N)$, $SU(N)$, $Sp(N)$). We study here this case and show that the algebraic structure can help in defining a sensible regularization scheme. We solve the parameterization problem of compact manifold that is responsible for singularities anytime that one wishes to describe in one coordinate system a compact manifold. The proposed solution defines a coordinate-free diffusion process accompanied by an appropriate numerical scheme. We demonstrate this framework in few examples of S^1 feature space regularization which is known also as orientation diffusion.

IC/MP627/013: Novel matrix methods for internet-data mining.

Organiser: Lek-Heng Lim (Stanford University, USA)
Co-organiser: Anirban Dasgupta (Yahoo! Research, USA)
Co-organiser: Gene Golub (Stanford University, USA)
Co-organiser: Michael Mahoney (Yahoo Research, USA)

Classical matrix factorization techniques such as the LU, QR, EVD and SVD, or their variants, have been used with great success in various data analytic applications. These include information retrieval, text mining, bioinformatics, computer graphics, computer vision, product recommendations, etc. In the past few years, internet applications have thrown some new challenges to the numerical linear algebraists. Unprecedented features and problems inherent in internet data have rendered traditional matrix factorization techniques less effective. Some of the new issues that arise in internet data mining include:

(i) *prohibitively large data size*: internet data sets are often much too large to allow multiple random accesses;
(ii) *massively incomplete data*: a significant proportion of the data may be missing;
(iii) *novel structures in data*: most importantly, datasets whose underlying structure cannot be adequately unraveled by LU, QR, EVD or SVD have become increasingly common, not just in internet applications but also in other scientific and engineering fields.

In the last few years, several new matrix factorizations have been proposed to deal with these issues. Some notables ones include: 1. Nonnegative Matrix Factorization (NMF); 2. Maximum Margin Matrix Factorization (MMMF); 3. Matrix Subspace Factorization (CUR); 4. Sparse Overcomplete Decoding (SOD). The key difference between these and the classical matrix factorizations is that they are not *rank-revealing* in the traditional sense but instead they *reveal* other properties of the structure under consideration. This minisymposium will focus on the development of these and other novel matrix computational tools with a view towards internet data mining applications.

Random sampling in large matrices. **Ravi Kannan** (Yale University, USA) IC/MT3985/013

Best low rank approximations of matrices are found by Singular Value Decomposition. For very large matrices, good low rank approximations can be found much faster and with less Random Access storage using the recently developed CUR decomposition. Here C is a (small) random subset of columns of the given matrix A, R is a (small) random subset of rows and U is found from C,R. Under a judicious choice of sampling probabilities, it can be shown that CUR aproximates any given A well. Besides, it is interpolative (in that C,R are sub-matrices of A) and this is useful in scientific applications. The talk will also describe some more recent work on improving the CUR approximation to acheive small relative error with respect to the best approximation. Extensions to tensors and combinatorial applications will be described as well. The talk is partly a survey about the work of many people.

New fast algorithms for non-negative matrix factorization. **Ming Gu** (UC Berkeley, USA) IC/MT4928/013

We present new fast algorithms for computing the nonnegative matrix factorizations. Our algorithms are based on interior point methods for solving linear programs. We show a special matrix structure in the Schur complement matrix associated with the interior point methods. We further develep an efficient algorithm based on exploiting such matrix structures.

This is joint work with Gene Golub and Lek-Heng Lim.

Combinatorial Laplacian and rank aggregation. **Yuan Yao** (Stanford University, USA), Lek-Heng Lim (Stanford University, USA) IC/MT5022/013

A graph is a 1-dimensional simplicial complex and the graph Laplacian is its corresponding 0-dimensional *combinatorial Laplacian*. Graphs and graph Laplacians have well-known and important applications in computer science in general and in machine learning in particular. While higher-dimensional simplicial complexes and combinatorial Laplacians have often played important roles in discrete and computational geometry, they remain relatively unknown and unused in machine learning. In this paper, we will attempt to convince the reader that machine learning theorists and practitioners should also be interested in the higher-dimensional combinatorial Laplacian, and in particular, the 1-dimensional combinatorial Laplacians (on 1- or 2-dimensional simplicial complexes). These arises naturally when one studies the rankings of objects by different people. In this context, the 1-Laplacian is a surprisingly effective tool—among other features, it allows one to aggregate distinct rankings, resolve inconsistencies, deal with incompletely rankings, and incorporate cardinal information. The main result that we employ is a discrete version of the Hodge Decomposition Theorem. In graph theory or linear algebra, this is simply an orthogonal decomposition of weighted directed graphs or skew-symmetric matrices. In physics, this is the decomposition of an electric field into curl free, divergence free, and harmonic parts. When suitably applied to the problem of rank aggregation, we obtain an orthogonal decomposition of ranking data into a *consistent* component and an *inconsistent* component—with a further decomposition of the consistent component into a *global* (consistent acyclic) component and a *harmonic* (consistent cyclic) component. These are then used to deduce useful information from the ranking data.

Page-rank by basis pursuit. **Michael Saunders** (Stanford University, USA), Sou-Cheng Choi (Stanford University, USA) IC/MT4008/013

The PageRank eigenvector is sparse in the sense that most elements are extremely small. Basis Pursuit is a reasonable tool for finding the tiny proportion of significant non-zeros.

IC/MP627/013: Novel matrix methods for internet-data mining. #2

Organiser: Lek-Heng Lim (Stanford University, USA)
Co-organiser: Anirban Dasgupta (Yahoo! Research, USA)
Co-organiser: Gene Golub (Stanford University, USA)
Co-organiser: Michael Mahoney (Yahoo Research, USA)

(For abstract, see session #1 above.)

An empirical meta-analysis for combining dependent hypothesis tests. **Art Owen** (Stanford University, USA) IC/MT3887/013

This work looks at combining several dependent statistical tests on related hypotheses. The motivating problem is a microarray experiment with $40 \times 16 \times 8932$ numbers. The goal is to identify which of 8932 genes are consistently related to aging in a subset of 16 tissues based on data from 40 individuals. The 16 test statistics for each gene are correlated. But patterns among the 8932 16-tuples may be used to estimate this correlation structure.

The Internet data mining connection is as follows: Similar problems arise in ecommerce and other fraud detection settings. There each entity suspected of fraud may be tested in multiple ways with the greatest suspicion falling on those that trigger multiple tests. Once again one has to combine dependent tests.

This work explains in detail some data analysis methods to be reported in a paper by Zahn *et al.* done in the Kim lab at Stanford University.

Maximum-margin matrix factorization. **Nathan Srebro** (Toyota Tech. Inst. at Chicago, USA) IC/MT3946/013

Factor, or linear component (PCA), models are often natural in the analysis of many kinds of tabulated data (e.g., collections of documents or images, gene expression measurements and user preferences). The premise of such models is that important aspects of the data can be captured by a small number dimensions (*component*,*factor* or *topics*).

I will present recent work on a novel approach that allows an unbounded (infinite) number of factors. This is achieved by limiting the norm of the factorization instead of its dimensionality. The approach is inspired by, and has strong connections to, large-margin linear discrimination. Unlike learning a low-rank factorization, learning a max-margin matrix factorization is a convex optimization problem that can be expressed as a semi-definite program, and I will discuss recent work on efficiently solving the resulting program, even on inputs with millions of observations. I will also discuss max-margin (low norm) factorizations and traditional low-rank factorizations as different measures of matrix complexity, and investigate the relationships between them.

I will use collaborative prediction (predicting unobserved entries of a partially observed matrix of user preferences) as an example application, and show how max-margin matrix factorizations are superior to previously suggested factorization methods for this task, and can achieve state-of-the-art prediction performance.

This is joint work with Alexandre d'Aspremont, Tommi Jaakkola, Jason Rennie, Adi Shraibman, Noga Alon and Sam Roweis.

Sampling-based algorithms for general regression problems. **Petros Drineas** (Rensselaer Polytechnic Institute, USA) IC/MT3956/013

ℓ_p regression algorithms have found numerous applications in many scientific domains. In this talk, we will argue that in the overconstrained case (i.e., given d variables and n constraints with n much larger than d), one can sample a small number of constraints and solve the induced problem in order to get relative error approximations to the original problem. The number of constraints to be sampled is a function of d and p. Particular emphasis will be placed on ℓ_1 and ℓ_2 regression problems.

Semi-nonnegative matrix factorization (NMF) and data clustering. **Chris Ding** (Lawrence Berkeley National Laboratory, USA) IC/MT3967/013

We show that the objective of NMF $X = FG'$ is equivalent to K-means clustering: G is cluster indicator and F contains cluster centroids. This can be generalized to semi-NMF where X, F contain mixed-sign data, with G being non-negative. We further propose convex-NMF by restricting $F$to be convex combinations of data points, ensuring F to be meaningful cluster centroids. We also show that the symmetric NMF $W = HH'$ is equivalent to Kernel K-means clustering and the Laplacian-based spectral clustering. All these follow by rewriting K-means objective as a trace of quadratic function whose continuous relaxation solution are given by PCA components. We emphasize orthogonality and nonnegativity in matrix based clustering. We derive the updating algorithms for semi-NMF, convex-NMF, symmetric-NMF and prove their convergence. We present experiments on face images, newgroups, web log and text data to show the effectiveness of these NMF based clustering.

Based on joint work with Xiaofeng He, Horst Simon, Tao Li and Michael Jordan.

IC/MP144/013: Laplacian eigenfunctions and their applications.

Organiser: Naoki Saito (UC Davis, USA)
Co-organiser: Mauro Maggioni (Duke University, USA)

Laplacian eigenfunctions have been successfully used in a variety of fields, such as image analysis, machine learning, data mining, computer graphics, and approximation theory. They are flexible to deal with high dimensional data with a lower-dimensional stochastic geometric structure. Moreover, together with the corresponding eigenvalues, they carry important geometric information about the domain where the data are sampled. The importance of the Laplacian eigenfunctions can be easily recognized by noticing that complex exponentials (or sines or cosines depending on the boundary conditions), spherical harmonics, and Bessel functions are in fact Laplacian eigenfunctions for specific canonical domains.

In this minisymposium, we shall showcase a variety of important and interesting applications employing Laplacian eigenfunctions and promote closer interactions among different communities listed above.

Laplacian eigenfunctions in geometry processing. **Bruno Levy** (INRIA Lorraine, France) IC/MT2916/013

The Laplacian operator plays an important role in Geometry Processing, as explained in the series of articles by Gabriel Taubin published at the Siggraph conference in the 90's. In this talk, we review the role of the eigenfunctions of this operator, by establishing the connections between existing works in various disciplines, comprising graph layout, dimension reduction, mesh parameterization, and more recent works on mesh quadrangulation. The talk is based on an article that we presented in the IEEE Shape Modeling International conference in 2006.

Can one hear shape?. **Martin Reuter** (Massachusetts Institute of Technology, USA) IC/MT850/013

The question "Can one hear the shape of a drum" has been asked in several contexts before (e.g., by Bers and Kac). It is a pictorial way of asking if the eigenvalues of the Laplacian on a given domain completely characterize its shape, in other words, if the spectrum is a complete shape descriptor (which it is not in general).

In this talk we will give an overview on how the computation of the spectra can be accomplished using FEM for manifolds in 2D and 3D (e.g. iso-surfaces, boundary representations, solid bodies, vector fields...) with the Dirichlet and Neumann boundary condition. We demonstrate that it is computational feasible to numerically extract geometric properties (volume, area, boundary length and even the Euler characteristic) from the first eigenvalues. Since the spectrum contains geometrical information and since it is an isometry invariant and therefore independent of the object's representation, parametrization, spatial position, and optionally of its size, it is optimally suited to be used as a fingerprint (Shape-DNA) in contemporary computer graphics applications like database retrieval, quality assessment, and shape matching in fields like CAD, medicine or engineering.

Laplacian eigen-maps as a tool for data analysis. **Mikhail Belkin** (Ohio State University, USA) IC/MT1346/013

I will discuss the importance of understanding geometry in various problems of data analyisis. Specifically, I will talk about the role of the Laplace-Beltrami operator as a key object associated to a Riemannian manifold, its usefulness for various tasks of data analysis and inference, and the problem of reconstructing the Laplace-Beltrami operator from sampled data.

Diffusion analysis of and on graphs, and high-dimensional data. **Mauro Maggioni** (Duke University, USA) IC/MT1143/013

We discuss ideas and constructions for the organization of graphs and data sets, based on random walks and diffusion processes on sets. One can generalize of Fourier and wavelet analysis to graphs and manifolds, leading to an organization of complex data sets and a generalization of signal processing tools to graphs. In order to emphasize the wide applicability of these techniques we will touch upon their applications to the organization of document corpora, dimensionality reduction for dynamical systems, nonlinear image denoising, semi-supervised and reinforcement learning.

IC/MP144/013: Laplacian eigenfunctions and their applications. #2

Organiser: Naoki Saito (UC Davis, USA)
Co-organiser: Mauro Maggioni (Duke University, USA)

(For abstract, see session #1 above.)

Laplacian eigenfunctions and physics Nobel prizes. **Lloyd Trefethen** (University of Oxford, UK) IC/MT2665/013

In recent years Timo Betcke and I have developed methods for high-accuracy computation of Laplacian eigenfunctions, building upon the method of particular solutions developed in the 1960s by Fox, Henrici and Moler here at the ETH. This talk will present some beautiful images resulting from these computations. It is remarkable how many physical phenomena can be seen in such results, and in particular, we shall relate Laplacian eigenfunctions to the Nobel Prizes in Physics awarded in 1902, 1903, 1907, 1909, 1918, 1919, 1933, 1952, 1963, 1964, 1977, and 1981.

Quantum mushrooms, scars, and the high-frequency limit of chaotic eigenfunctions. **Alex Barnett** (Dartmouth College, USA), Timo Betcke (University of Manchester, UK) IC/MT2422/013

It is a long-standing question how eigenfunctions of the Laplacian in a cavity behave asymptotically at large eigenvalue, when the ray or 'billiard ball' dynamics (Hamiltonian motion of a point particle in the cavity) is chaotic. This field is called 'quantum ergodicity' or 'quantum chaos', and has applications to physics, chemistry, acoustics, and connections to number theory and automorphic forms. It is known that almost every eigenfunction tends to spatial uniformity, however the *rate* at which this occurs is unknown. I investigate these numerically, at mode numbers up to of order 10^6, using specialized global approximation methods. I find evidence for the Quantum Unique Ergodicity conjecture of Rudnick-Sarnak, and for an ergodicity rate conjecture of Feingold-Peres involving the classical autocorrelation. I will also discuss the debate over 'scarring' (ghosts of periodic ray orbits in the eigenfunctions), and present work with T. Betcke on cavities such as Bunimovich's mushroom which possess both chaotic and integrable motion.

Laplacian eigenfunctions: fast computation via commuting integral operators and applications to image analysis. **Naoki Saito** (UC Davis, USA) IC/MT2579/013

Laplacian eigenfunctions, as a generalization of the Fourier basis over a rectangular domain, allow us to perform spectral analysis of data recorded on a domain of general shape. Examples include cells in histological images and meteorological data sampled at weather stations. We will present a method to analyze such images by expanding them in terms of the Laplacian eigenfunctions defined over such general shape domains. Directly solving the associated Helmholtz equations on such domains or computing the Green's functions satisfying specific boundary conditions imposed on such domains are in general difficult. Instead, we find an integral operator commuting with the Laplacian without imposing strict boundary conditions *a priori*, and compute the eigenfunctions of this integral operator, which are in fact the Laplacian eigenfunctions. This approach is amenable to modern fast numerical algorithms. In particular, we will discuss two possible strategies. One is to use multiwavelets of Alpert to sparsify the kernel of this integral operator to speed up the computation. The other is to use

the Fast Multipole Method as a fast matrix-vector multiplication, which is indispensable for large scale iterative eigenvalue-eigenvector solvers such as the Lanczos iteration.
In addition, we will present applications of Laplacian eigenfunctions to statistical image analysis and contrast them with Principal Component Analysis.

Random computational tomography and protein structuring. **Amit Singer** (Yale University, USA) IC/MT4809/013

In this talk we present a reconstruction algorithm for the 3D atomic structure of randomly oriented proteins using modified graph laplacians. The 2003 Nobel Prize in Chemistry was co-awarded to R. MacKinnon who was the first to structure a protein channel (the potassium channel) in 1998 by crystallizing the protein and using the classical X-ray computed tomography (CT). However, most membrane proteins cannot be crystallized and the classical CT cannot be used. In our experimental setup, the data consists of thousands of real noisy 2D projections (electron microscope images) of the protein given in random unknown directions, because the proteins are randomly oriented rather than being aligned as in MacKinnon's setup. Still, we show that the reconstruction is made possible by a certain modification of the images' graph laplacian coupled with the 3D Fourier slice theorem. The reconstruction is a particular case of a more general spectral non-linear independent component analysis (ICA) algorithm that combines local principal component analysis (PCA) with the graph laplacian. No prior knowledge of graph laplacians, tomography and proteins is needed for this talk. This is a joint work with Ronald Coifman, Yoel Shkolnisky and Fred Sigworth (Yale University).

IC/MP298/014: The AIM@SHAPE digital shape workbench as an e-Science collaboration tool.

Organiser: Ewald Quak (Tallinn University of Technology, Estonia)

Developing and maintaining computational research software has become a more and more complex endeavour, especially when considering aspects like quality control, training of young researchers, exchange between different teams and also to avoid reinventing the wheel.
The EU IST Network of Excellence AIM@SHAPE (www.aimatshape.net) on 3D shape modelling involves ca. 200 researchers and graduate students, coming from 13 institutions in 8 countries. Application areas in the project include industrial design, the link between geometrical representations and numerical simulation software as well as the use of virtual humans.
One of the most important project goals is to develop a Digital Shape Workbench (DSW) as an international software infrastructure for research in 3D shape modelling using suitable ontologies. As a collaboration tool the DSW is meant to be freely accessible for researchers in the subject area, well beyond the consortium that is currently building it.

This minisymposium is one of the means to popularize the Digital Shape Workbench in the scientific community of potential users. Apart from a general introduction to the research infrastructure provided by the network, the use of the shape model and software tools repositories will be demonstrated. Also some examples for the role of the DSW in the research program of the network will be presented.

The AIM@SHAPE DSW: semantic-centric usage scenarios. **Manolis Vavalis** (ITI-CERTH, Greece) IC/MT1526/014

In this paper we present case studies where semantic technologies have the potential to be used to build robust real-life solutions out of the AIM@SHAPE Digital Shape Workbench both in its current and its future forms. The aim of this study is not to actually report on the success (or failure) of existing usage scenarios but to focus on understanding what makes semantic knowledge applications successful in operational environments which involve shapes.

Mathematical aspects involved in virtual human construction and simulation for industry. **Laurent Moccozet** (Université de Genève, Switzerland), Frederic Vexo (École Polytechnique Fédérale de Lausanne, Switzerland) IC/MT1871/014

Virtual Humans are more and more involved in Virtual Environments for various areas of applications in industry: ergonomics, training, video games ... For all these applications, sophisticated models that reproduce as closely as possible not only the shapes of real Humans but also their dynamic behavior and their interactions with the environment are required. Thanks to the combination of currently available shape and motion acquisition devices with geometrical shape analysis and processing tools, it becomes possible to define accurate virtual models with limited efforts.

Combining modeling, simulation, optimization and analysis under a unique framework. **Sebastian Pena Serna** (Fraunhofer-IGD, Germany), Andre Stork (Fraunhofer-IGD, Germany) IC/MT2460/014

The virtual engineering process has several phases and every phase needs special representations and/or tools. The process itself is complex and in addition, one has to deal with conversions, transformations and transitions between phases which consume time and therefore increase the complexity, the incompatibility and the expenses. On the other hand, the phase teams are not integrated because of this incompatibility and hence, new and advanced concepts, methodologies, approaches and applications cannot be defined in order to solve and support their needs and requests.

Hence, we are defining, designing and developing a framework where the phases of the virtual engineering process can be executed, integrated and combined without transitions or conversions. In order to achieve our target, we have chosen the mesh representation as the unique representation, because this is the most typical representation for 3D domains within the engineering analysis. Additionally, we are enriching the mesh with mathematical definitions which should allow for combining modeling, simulation, optimization and analysis under the same framework and therefore simplifying the virtual engineering process. This approach will support the engineers with advanced techniques on modeling meshes, conceptual simulations, real time optimization and more accurate analysis.

Contributions to robust scattered data denoising. **Oliver Schall** (Max-Planck-Institut Informatik, Germany) IC/MT1703/014

Many of today's applications make use of 3D data digitized from real-world objects such as machine parts, terrain data, and cultural heritage. In spite of recent progress in developing reliable methods for denoising scattered data, the quest for accurate, and adaptive denoising techniques capable of processing large and very noisy datasets remains a major research issue in computer graphics and geometric modeling.

In this talk, an overview of recent developments in scattered

data filtering will be given. Special attention will be paid to new denoising techniques developed within the AIM@SHAPE framework. In particular, contributions related to processing uncertain and time-varying data will be discussed.

IC/MP298/014: The AIM@SHAPE digital shape workbench as an e-Science collaboration tool. #2

Organiser: Ewald Quak (Tallinn University of Technology, Estonia)

(For abstract, see session #1 above.)

The AIM@SHAPE network of excellence and its research infrastructure for shape modelling. **Bianca Falcidieno** (Consiglio Nazionale delle Ricerche, Italy), Ewald Quak (Tallinn University of Technology, Estonia) IC/MT1533/014

This is the scene-setting introductory talk of this minisymposium. The scope of the AIM@SHAPE network is described and the network's general goal is addressed: to use techniques from knowledge technology, such as ontologies, in shape modelling research. An overview is given on the main tangible outcome of the project, namely the features of a lasting research infrastructure, accessible to the research community as a whole. The core element is formed by the AIM@SHAPE Digital Shape Workbench (DSW), where the necessary flow of interaction and communication is implemented that allows to access and to use the various software components developed and maintained by the project. The detailed use of the DSW and specific research results from the network are then described in the following lectures.

The AIM@SHAPE shape repository. **Waqar Saleem** (Max Planck Institut Informatik, Germany) IC/MT1935/014

In a space of a little over 2 years, the AIM@SHAPE Shape Repository has become one of the European reference databases for digital shape models. The repository is populated by AIM@SHAPE project partners with digital shape models that either reflect their ongoing research or are acquired exclusively for the repository. The repository itself is ontology-driven, i.e. stored models are categorized using the AIM@SHAPE Shape Common Ontology. The shape category then determines the necessary metadata that will accompany the model.

In my talk, I will present some background on the Shape Repository followed by a demo. I will first demonstrate how the Shape Repository meets all expectations a user may have from a standard online digital shape database, and then go on to its unique features. Finally, I will talk about how online users can help to improve it.

The AIM@SHAPE tool repository. **Laurent Saboret** (INRIA Rocquencourt, France), Pierre Alliez (INRIA Sophia Antipolis, France) IC/MT1519/014

The tool repository of the AIM@SHAPE Network of Excellence is an inventory of shared software that collects and documents a number of state-of-the-art tools that can be used at different stages of the digital shape lifecycle. In this talk we will present some of the tools at work in two scenarios. In the first scenario a physical shape is acquired using a laser scanner, processed, structured and semantically annotated. The second goes the other way around, from the semantic to the final geometric realization of a shape.

Bridging geometry and semantics: the AIM@SHAPE research perspective. **Michela Spagnuolo** (Consiglio Nazionale delle Ricerche, Italy), Jean-Claude Leon (Institut National Polytechnique Grenoble, France), Fatih Demirci (Universiteit Utrecht, The Netherlands) IC/MT2042/014

The scientific innovation sought by AIM@SHAPE is to move towards digital representations of shapes which are able to model not only the visual appearance of objects but also their meaning or functionality in a given knowledge domain.

While the technological advances in terms of hardware and software have made available plenty of tools for using and interacting with the geometry of shapes, the interaction with the semantic content of digital shapes is still far from being satisfactory. While we have tools for viewing digital shapes even in much unspecialised web contexts (e.g. browsers plugins like SVG or VRML for 3D shapes), we miss tools for interacting with the semantics of digital shapes.

If we want to move towards semantically capable digital representations of shapes, we have to put an entirely new perspective on the traditional modelling pipeline, trying to understand where and how the semantics can be encapsulated in the digital representation of shapes.

With this background, results and open issues will be presented mainly focused on the different stages at which it is necessary to formalize an interaction between the semantic and the geometric level of representation of 3D shapes, both in top-down and bottom-up pipelines of modelling.

IC/MP4421/014: Level-set methods: current development.

Organiser: Yen-Hsi Tsai (University of Texas at Austin, USA)

Several problems that arise in science and engineering can be formulated as a front evolution between two (or more) phases. Examples include solidification problems, dendritic growth in materials science, free surface flows, multiphase flows, to cite a few. One of the main the difficulties in solving such problems comes from the fact that the interface location must be computed as part of the solution to the underlying equations. Since their inception, level set methods have been extremely successful in tackling these problems. In this minisymposium, the focus will be given In this minisymposium the focus will be given to recent advances in the core level set algorithms as well as their applications. Specifically, the core algorithm will cover topics on adaptivity, volume conservation, and solving inverse problems. Applications will include multiphase flows, high frequency wave propagation and shape optimization. This minisymposium will offer an excellent opportunity for researchers to learn about a wide variety of recent developments in the computational aspects of level set methods as well as their applications and will stimulate cross-pollination between disciplines.

Computational high-frequency waves through barriers or interfaces. **Shi Jin** (University of Wisconsin, Madison, USA) IC/MT1344/015

We introduce Eulerian methods that are efficient in computing high-frequency waves through barriers or interfaces. The method is based on the classical Liouville equation in phase space, with discontinous Hamiltonians (or singular coefficients) due to the barriers or material interfaces. We provide physically relavant interface conditions consistent with the correct transmissions and reflections, and then build the interface conditions into the numerical fluxes. This method allows the

resolution of high frequency waves without numerically resolving the small wave lengths, and capture the correct transmissions and reflections at the interface. Moreover, we extend the method to include diffraction, and quantum barriers. Applications to semiclassical limit of linear Schrödinger equation, geometrical optics, elastic waves, and semiconductor device modeling, will be discussed.

Discrete δ-functions concentrated on level sets. **Peter Smereka** (University of Michigan, Ann Arbor, USA) IC/MT1173/015

It is shown that a discrete delta function can be constructed using a technique developed by Anita Mayo for the numerical solution of elliptic equations with discontinuous source terms. This delta function is concentrated on the zero level set of a continuous function. In two space dimensions this corresponds to a line and a surface in three space dimensions. Delta functions that are first and second order accurate are formulated in both two and three dimensions in terms of a level set function. The numerical implementation of these delta functions achieves the expected order of accuracy.

Discretizing δ functions supported on level-sets. **John Towers** (MiraCosta College, USA) IC/MT1350/025

I will explain how an effort to solve a certain parabolic free boundary problem related to flame propagation resulted in some new methods for computing delta functions supported on level sets. For the purpose of computing an integral over a manifold of codimension one defined by a level set, these methods yield approximations that are accurate, have relatively small bandwidth, and are known to be convergent. The one-dimensional version of one these algorithms also seems to be well suited to approximating the type of singular integral that arises when computing multivalued observables for the semiclassical limit of the Schrödinger equation (with one space dimension) using the level set method. In more than one spatial dimension, this problem requires the calculation of singular integrals of higher codimension, possibly requiring a different technique. I will report on progress toward extending this technique, and a new technique that exploits the full codimension aspect of the problem, to these singular integrals.

Geometry-aware discretizations of level-set methods: application to tumor growth. **John Lowengrub** (University of California, Irvine, USA) IC/MT3247/015

An advantage of using level set methods for moving boundary problems is that geometric quantities such as curvature can be readily calculated from the level set function. However, in topologically challenging cases (e.g., when two interfaces are in close contact), level set functions develop singularities that yield inaccuracies when using traditional discretizations. In this talk, we discuss improvements to the algorithms such that second order accuracy is achieved near transitions. We then develop a 2nd order accurate level-set/ghost-fluid algorithm for use with mathematical models of solid tumor growth. A novel feature of this algorithm is the accurate treatment of normal jumps across the interface.

IC/MP4421/014: Level-set methods: current development. #2

Organiser: Yen-Hsi Tsai (University of Texas at Austin, USA)

(For abstract, see session #1 above.)

A hybrid coupling interface method for elliptic complex interface problems. **Yu-Chen Shu** (National Taiwan University), I-Liang Chern (National Taiwan University) IC/MT3855/025

In dealing with elliptic *complex* interface problems, most finite-difference methods under Cartesian grid fail due to their restrictions to the interfaces for the purpose of interpolation. In this paper, we first propose a first-order coupling interface method (CIM1) in any dimensions which uses only the standard nearest neighboring grid data. It only requires that each grid segment (the segment connecting two adjacent grid points) intersects the interface at most once. As a result, it is robust and flexible to handle complex interface problems.

Next, we propose a hybrid coupling interface method (hybrid CIM) to get higher order accuracy for handling elliptic complex interface problems in arbitrary d dimensions. We classify the underlying Cartesian grid points into interiors, normal on-fronts and exceptionals. Standard central finite difference is used at interior grid points. A second-order coupling interface method (CIM2) proposed in our previous paper is adopted at those normal on-front points. The CIM1 is applied at the exceptional points. This hybrid coupling interface method maintains second order accuracy in most applications due to the fact that usually the number of normal on-front grid points is $O(h^{1-d})$ and the number of the exceptional points is $O(1)$.

We compare our hybrid CIM with other interface method that handle complex interface problems in two dimensions, our method is robust and produces less errors. In addition, we perform several numerical tests in three dimensions. The results show that the hybrid CIM can maintain second order accuracy for complex interface problems.

Conjugate-gradient and quasi-Newton methods for level-set-based shape-optimization problems. **Wolfgang Ring** (Universität Graz, Austria) IC/MT4252/015

The nonlinear conjugate-gradient method and the class of quasi-Newton methods are typical examples of optimization techniques which rely on the vector space structure of the set of optimization variable. For the CG-method, the descent direction is constructed as $p_{k+1} = -\nabla f_{k+1} + \beta_k p_k$ i.e. a linear combination of the gradient direction in the current point and the descent direction in the previous point. Similarly, quasi Newton method use finite differences of gradients in the current and the previous point for the construction of the approximate Hessian. When applying these ideas to the solution of shape optimization problem, one faces the difficulty that shapes are not elements of a vector space (at least not in a straight forward way), and hence the update formulas have to be modified. We suggest to use the level-set method for the transport of information between successive iterates produces by the optimization algorithm.

Inverse problems involving shapes. **ChiuYen Kao** (The Ohio State University, USA) IC/MT3386/015

Identification or optimization of shapes arises in many science and engineering applications. Recently shape derivatives and topological derivatives have been incorporated into level set method to study inverse problems involving shapes. This talk will provide an integrated introduction to the basic definition of shape derivatives and topological derivatives, and the combination with level set methods in a descent framework. Finally, specific applications for identifying shapes of drums and optimization of quality factor are presented.

Existence and uniqueness of level sets for spiral crystal growth. **Takeshi Ohtsuka** (Sophia University, Tokyo, Japan) IC/MT3957/015

The aim of this talk is to propose a new level-set approach for spirals.

In 2003, I adjusted the level-set formulation for the spiral crystal growth, and prove the existence and uniqueness of viscosity solutions for a level set equation. The formulation reflects an idea of R. Kobayashi who introduced a kind of Allen–Cahn formulation for the spiral crystal growth. To complete the strategy to obtain spiral curves by this level set formulation, we see the uniqueness of level sets and construct an initial datum by initial curves.

To prove the uniqueness, we adjust the way to prove the uniqueness for the usual level set formulation due to Y.-G. Chen, Y. Giga, and S. Goto, and L.C. Evans and J. Spruck. Their strategy is to use the comparison principle and the rescaling invariance of solutions for geometric equations. However, the level set equation for spiral crystal growth is not geometric. To overcome this difficulty, we introduce a new rescaling of dependent variables which represents dislocation as a level set, and its invariance. I also show the way to construct an initial datum in several simple cases and the result of numerical computation.

Computing, Contributed Talks

IC/CTS4656/01: **Computing miscellaneous, II.**

Organiser: Akambadath Keerthiyil Nandakumaran (Indian Institute of Science Bangalore)

Quasi-Newton algorithm for best multi-linear rank approximation of tensors. **Berkant Savas** (Linköpings universitet, Sweden) IC/CT4745/015

In this talk we introduce a novel method for solving the best multilinear rank approximation problem. Our algorithm differs from existing methods in two respects: (1) it exploits the fact that the problem may be viewed as an optimization problem over a product of Grassmann manifolds; (2) it uses Quasi-Newton-like Hessian-approximates specially adapted for Grassmannians and thus avoids the inevitable problem of large Hessians in such problems. Tensor approximation problems occur in various applications involving multidimensional data. The performance of the Quasi-Newton algorithm is compared with the Newton-Grassmann and Higher Order Orthogonal Iteration algorithms for general and symmetric 3–tensors.

Methods and a system of functional programming for supporting supercomputing. **Victor Kasyanov** (Institute of Informatics Systems, Russian Federation) IC/CT472/015

In the paper the SFP project being under development at the Institute of Informatics Systems in Novosibirsk is considered.

The SFP system is intended to be a visual interactive programming environment that simplifies construction of correct parallel programs by isolating the programmer from the complexities of parallel processing and supports development of high quality, portable software for parallel computers on low cost, sequential computers (PC).

The SISAL 3.0 language that has been designed as the input language of SFP supports annotated functional programming, exposes implicit parallelism through data dependence and guarantees determinate result.

The SFP system uses intermediate languages of hierarchical graphs and provides means to write and debug SISAL-programs regardless target architectures as well as to translate the SISAL-programs into optimized imperative programs, appropriate to the target execution platforms.

The author is thankful to all colleagues taking part in the SFP project. The work is partially supported by the Russian Foundation for Basic Research (under grant N 07-07-00056).

Soft-fuzzy computing and modelling. **Witold Kosiński** (Polish-Japanese Inst./Kazimierz Wielki University, Poland) IC/CT3099/015

In real-life problems both parameters and data used in mathematical modelling are *vague*. The vagueness can be described by fuzzy numbers and sets. Pattern recognition, system modelling, diagnosis, image analysis, fault detection and others are fields where soft calculation with unprecise, fuzzy objects plays an important role. In the paper a short review of recent results in the theory of ordered fuzzy numbers and their normed algebra is given.

Ordered fuzzy numbers are generalizations of *convex* fuzzy numbers that make possible to deal with fuzzy objects exactly in the same way as with real numbers. They form a Banach space, partial ordered ring and even more a *commutative Banach algebra* with unity. Linear and bounded functionals which form a large class of *defuzzyfication operators* are represented here by sums of two Stieltjes integrals with respect to functions of a bounded variation. An approximation formula of a general nonlinear defuzzyfication operator is also derived.

Specific applications in finance, dynamical systems and mechanics are presented. From the classical framework known algebraic and evolution equations describing such systems are transformed into their fuzzy versions. Their solvability is shortly presented together with the specially dedicated problem solutions.

Direct reconstruction of complex refractive-index distribution. **Akambadath Keerthiyil Nandakumaran** (Indian Institute of Science Bangalore) IC/CT4275/001

Diffraction tomographic reconstruction of refractive-index distribution requires complete knowledge of the transmitted complex field at the boundary. Here we present a method which can reconstruct the complex refractive index distributions from intensity-based measurements which are logarithm of intensity and the normal derivative of intensity. We have presented an iterative algorithm which requires efficient implementation of a forward wave propagation equation and sensitivity matrices for the above two type of measurements. An efficient method for estimation of the sensitivity matrices is given and also the forward operator. The results of numerical experiments show that the two data types, namely $log(I)$ and $\frac{\partial I}{\partial n}$ reconstruct respectively the imaginary and real part of the refractive index distribution. The forward operator, a Helmholtz equation, is implemented for small k(k=50 in our example). As a consequence, the reconstructed inhomo-

geneities are spread and smoothened. Implementation of the Helmholtz equation for large k requires very fine meshing which pushes up computation and numerical instability. For the present method to be applicable in optical refractive index reconstruction an accurate and efficient forward solver for large k is required. This is currently being attempted using a wavelet-based, multi-scale procedure.

A novel two-factor forecasting model for fuzzy time series. **Sheng-tun Li** (National Cheng Kung University, Taiwan), Su-Yu Lin (National Cheng Kung University, Taiwan), Yi-Chung Cheng (National Taiwan Normal University) IC/CT4271/013

Recently, the forecasting model of fuzzy time series has attracted a lot of interests since it is capable of dealing with vague and incomplete time series data represented as linguistic values under uncertain circumstances. In this paper, we propose a novel two-factor forecasting model for fuzzy time series. In contrast to related work, the proposed model can reduce the computation complexity without deriving all fuzzy logic relationships in advance. Moreover, it can overcome the hurdle of determining the k-order issue in other high order models. A fuzzy C-means clustering algorithm is utilized in fuzzifying and partitioning intervals for the historical data. Experimental results demonstrate that our model not only achieves the better accuracy with the mean square error and average forecasting error rate than previous models, but also is considered as robustness under a simple Monte Carlo simulation. The consistency performance about the number of intervals is coincided with the principle that the more the number of intervals is, the better the forecasting accuracy is achieved.

IC/CTS4653/01: Computing miscellaneous, I.

Organiser: Yannis Kalaidzidis (Max-Planck-Institut Dresden, Germany)

Fast 3D surface-mesh denoising with edge preservation and mesh regularization. **Hui Huang** (University of British Columbia, Canada), Uri Ascher (University of British Columbia, Canada) IC/CT4259/012

We describe a hybrid algorithm that is designed to smooth, but not only smooth, noisy polygonal surface meshes with sharp edges. While denoising, our method simultaneously regularizes triangle meshes on flat regions for more advanced processes and preserves edge sharpness for authentic visualization. A clustering technique, which combines K-means and spectral clustering methods, is first developed according to our specific geometry prior. It is then used to implement vertex classification so that we can subsequently apply different smoothing operators on different vertex groups. This yields a highly efficient robust algorithm that is capable of handling both edge sharpness and mesh sampling irregularity without any significant cost increase.

Towards a high-content analysis of high-throughput imaging data: multiparametric analysis of siRNA phenotypes and their reproducibility. **Yannis Kalaidzidis** (Max-Planck-Institut Dresden, Germany) IC/CT4691/000

One key challenge of the post-genomic era in biology is the elucidation of gene functions and the mechanistic understanding of cellular processes in which the genes participate. Gene silencing by means of siRNA/esiRNA knockdown in conjunction with high-throughput microscopy-based readouts offer a promising approach. However, the large degree of morphological variation between cells in an image frame represents a major challenge to the reliable identification of siRNA-phenotypes. At present, most high-throughput imaging experiments have therefore resorted to an almost qualitative readout. Is the cell infected? Is the cell cycle blocked?. Accessing the quantitative information in the image sets would be desirable both in reducing the number of false negatives as well as allowing more accurate classifying phenotypes. Using the sub-cellular distribution of endosomal organelles as assay, we have developed a system for the high-content analysis of automatically-acquired high-resolution images. More than 10 parameters describing the intra-cellular distribution of endosomal organelles in quantitative terms were developed. The stability of parameters was tested by calculation the correlation between different imaging sessions and between experimental replicates. The analysis showed that different parameters reveal a wide variation of stabilities which dependent on biological variability, typical automatic imaging problems and parameter calculation details. The comparison of parameters stability between different siRNAs targeting the same gene with respective stability between different replicates provides a tool for establishing the phenotype reproducibility by siRNA technology. Statistical analysis of these data will be of critical importance in establishing objective phenotype definitions and thus for the experimental design of the next generation of high-content screens.

Software engineering for numerical simulation of 2D non-stationary real MGD flows. **Livio Maglione** (Universidad Nacional de Río Cuarto, Argentina), Sergio Elaskar (Universidad Nacional de Córdoba, Argentina), Hector Brito (Universidad Nacional de Río Cuarto, Argentina), Raul Dean (Universidad Nacional de Río Cuarto, Argentina), Luis Lifschitz (Universidad Nacional de Río Cuarto, Argentina) IC/CT3381/010

The study of flows in which a electrically conducting gas moves in a magnetic field is known as magnetogasdynamics or MGD for short. Computational MGD represents one of the most promising interdisciplinary computational technologies for aerospace design. At the present, in Argentina, it is being developed an ablative magnetoplasmadynamic thruster (AMPD) as a native propulsion option for satellite and, particularly, microsatellite orbit and/or attitude control.

A MGD model is generally based on the assumption that plasma can be regarded as a continuum and thus may be characterized by relatively few macroscopic quantities. A model for a flow affected by electromagnetic forces includes the full set of Maxwell's equations coupled with the Navier–Stokes equations. The real MGD equations constitute a parabolic–hyperbolic partial differential system. In addition the ideal part of the MGD equations is nonconvex and as consequence the wave structure is more complicated than for the Euler equations.

A software engineering was developed and using structured meshes solves 2D, time-dependent, viscous and resistive MGD flows. In this case, the numerical approach consists of an approximate Riemann solver coupled with the TVD scheme proposed by Yee. The eigensystem introduced by Powell and the normalization of the eigenvectors presented by Zarachay *et al.* have also been used.

To check accuracy, the computational code has been applied in the simulation of a Riemann problem introduced by Brio and Wu. Also results in the simulation of the Hartmann flow are shown. The results obtained are in good agreement with those reported by other authors.

Adaptive numerical simulation of intracellular calcium dynamics. **Nagaiah Chamakuri** (Universität Magdeburg, Germany) IC/CT5065/012

In my talk I will present the adaptive numerical simulation of intracellular calcium dynamics. Calcium is an important second messenger in cell communication. The dynamics of intracellular calcium is determined by the liberation and uptake by cellular stores as well as reactions with buffers. We develop models and numerical tools to study the liberation of calcium from the endoplasmic reticulum (ER). This process is characterized by the existence of multiple length scales. The modelling of diffusion, binding and membrane transport of calcium ions in cells leads to a system of reaction-diffusion equations. We used piecewise linear finite elements for the spatial discretization and time discretization by a linearly implicit Runge–Kutta scheme. In our description the dynamics of IP3-controlled channels remains discrete and stochastic. The strongly localized temporal behaviour due to the on-off behaviour of channels as well as their spatial localization is treated by an adaptive numerical method. We present sequential and parallelized numerical results.

IC/CTS4652/01: Data analysis and visualisation.

Organiser: John Bowman (University of Alberta, Canada)
Co-organiser: Toshinori Munakata (Cleveland State University, USA)

The 3D-asymptote generalization of the MetaPost Bézier interpolation algorithms. **John Bowman** (University of Alberta, Canada) IC/CT3271/013

The descriptive vector graphics language Asymptote provides for the typesetting of mathematical figures a capability analogous to what TEX provides for typesetting equations (http://asymptote.sourceforge.net/). It was inspired by Hobby's MetaPost (a modified version of MetaFont, the program that Knuth wrote to produce the TEX fonts) but features a more elegant C++-like syntax, high-order functions, and robust floating-point numerics. Labels are typeset with TEX, for professional quality and overall document consistency, and the simplex linear programming method is used to solve overall size constraint issues between fixed-sized and scalable objects.

Asymptote generalizes to three dimensions the prescription of Hobby (Discrete and Computational Geometry **1**, 1986) for drawing an aesthetically pleasing, numerically efficient, interpolating spline given a set of nodes and optional tangent directions. This generalization is shown to be shape-invariant under three-dimensional rotation, scaling, and translation, and reduces in the planar case to Hobby's prescription. Both the nodes and control points of the three-dimensional Bezier curves are projected to two-dimensional Bezier curves.

Asymptote was designed to generate native Postscript and PDF output since these are the portable standards understood by professional printers. However, Postscript and PDF support only Bezier splines, which are invariant under orthographic (affine) but not perspective projection. Since non-uniform rational B-splines, which are invariant under perspective projection, cannot be reduced to Bezier splines without loss, it is important to consider the error introduced by using three-dimensional cubic Bezier splines for perspective drawings.

Given that all Metapost and Asymptote guarantee is that the path passes through a set of nodes, respecting any explicit tangent and straightness conditions, we argue that, in practice, the error inherent in using Bezier splines for drawings with perspective distortion is as acceptable as the usual 0.06% accurate 4-node Bezier approximation to a circle. In both cases, one can always specify additional nodes and control points to obtain any desired graphical accuracy.

The reassignment method with the Stockwell transform. **Cheng Liu** (York University, Canada) IC/CT2551/013

Instantaneous frequency (IF) is a critical parameter in describing non-stationary signals whose frequency characteristics vary over time. In real application, it is usually difficult to obtain accurate IF estimation of signals in terms of their multi-component feature and the presence of noise. The reassignment method provides a technique to obtain a more concentrated IF representation by re-locating the original information of time-frequency representation. In this talk, we will extend the reassignment method with the recently developed time-frequency representation: the Stockwell transform. The improvement of our new methodology is shown by numerical simulations.

Constraint isomorphism and correction algorithms for violations. **Toshinori Munakata** (Cleveland State University, USA), Adam Fadlalla (Cleveland State University, USA) IC/CT1736/013

In many domains such as science, engineering and operations research, a problem is characterized in terms of different parameter sets. A constraint imposed in terms of a parameter in one parameter set must be consistent with a constraint in another parameter set. We call such consistency among parameter sets *constraint isomorphism* [1]. When mapping among the parameter sets is not so visibly obvious, one might overlook consistency violations, which have occurred in the past. Constraint isomorphism is important in many situations, including generation of random data for simulation of stochastic problems.

As a case study we consider the total tardiness problem, an NP-complete job scheduling problem. Two parameter sets are commonly employed for this problem. For easy reference, we call one set "data parameters" and the other "characteristic parameters." Processing time and due date for each individual job are data parameters, and the tardiness factor τ and relative range of due dates δ are characteristic parameters. For the simplest, single machine model, each job is processed by the single machine at a time. n jobs wait for processing at time t = 0, and they have *processing times* p_1, p_2, ..., p_n, and *due dates* d_1, d_2, ..., d_n, respectively. The objective of the problem is to determine the order of jobs to be processed to minimize the *total tardiness*. Extensive works have been performed for the tardiness problem, employing various methods. A common scenario is that each of the τ and δ values is selected from a set of numbers. It has been shown that some of these selected pairs yield two types of violations: 1. Non-negative due date. The due date for every job must be non-negative, that is, $d_i \geq 0$. 2. Due date $\geq$ processing time for every job, i.e., $d_i \geq p_i$.

We present several algorithms to remove these violations. They include: discard-and-replace, modified probability distributions, and data-interchanging. The upper bound of the computational complexity of the last algorithm is O(*mn* log (*mn*)), where m is the number of problems in the entire problem set under consideration.

Reference

[1] Munakata, T. and Fadlalla, A. Constraint isomorphism and the generation of stochastic data, *IIE Transactions*, 38 (2006), 437-444.

Data-uncertainty analysis in environmental management. **Michal Hejc** (Masaryk University, Czech Republic), Jiri Hrebicek (Masaryk University, Czech Republic) IC/CT2857/013

Imprecision of data is an important characteristic feature of environmental monitoring, particularly at all kinds of fixed and moving sensor networks. When making evaluations, conclusions and the decisions from collected data, we have to assess data quality not to make fatal mistake. The important task of computing and current information management is to deal with the primary data uncertainty and using knowledge about data quality to assure the new architecture is generic enough and provides added value for the end users. This will reduce the risk of wrong decision in environmental management. At present new approaches and methodologies to handle environmental data uncertainty are explored as opposite to standard. The paper presents comparison of such new approach against European Environment Agency and U.S. Environmental Protection Agency standards in the several cases of the assessment of environmental management indicators in the Czech Republic. The new approach to information management with data quality assessment brings more flexible way of dealing with all kinds of uncertainty. There are presented better results and less workload then standard approach in the paper.

Markovian model of genetic algorithms and its asymptotic behaviour. **Witold Kosiński** (Polish-Japanese Inst./Kazimierz Wielki University, Poland), Stefan Kotowski (Polish Academy of Sciences, Poland) IC/CT3106/011

In the last time there has been growing interest in universal optimization algorithms, which use only limited knowledge about problems to be solved and are constructed on the basis of some similarity to processes realized in nature. Between them are *genetic algorithms* which perform a multi-directional search by maintaining a *population* of potential solutions and encourages information formation and its exchange. A population undergoes a simulated evolution due to the iterative action with some probability distributions of a composition of three operators: *mutation, crossover and selection*. If we imagine that a population is a point in the space Z of (encoded) potential solutions then the effect of one iteration of this composition is to move that population to another point.

In our analysis first we are concerned with probability distributions of each population for a particular case of the simple genetic algorithm (SGA) in which crossover is not present and then we admit for adaptation of algorithm parameters during the evolution. In SGA with known fitness function the *proportional selection* and the mutation allow to write the probability distribution for the next population in the form of the multiplication of two matrices times the population (frequency) vector. Finally the composition of both operations leads to the general form of the *transition operator* (matrix) acting on a new probability vector representing a probability distribution of appearance of all populations of the same *size*. The matrix appearing there turns to be Markovian and each subsequent application of SGA is the same as the subsequent composition of that matrix with itself. Thanks to the well-developed theory of Markov operators new conditions for the *asymptotic stability*: general and point-wise of the transition operator, are formulated. The case of different selection operators is also treated.

Computing, Posters

IC/PP3894/012: Application of the R-functions method to the solution of the Poisson equation.

Presenter: Svyatoslav Gladkov (Universität Dortmund, Germany)
Co-author: Bob Svendsen (Universität Dortmund, Germany)

Present-day solution techniques for partial differential equations (PDEs) in more than one dimensions require the use of various spatial discretization schemes like finite elements method (FEM) or boundary elements method (BEM). But for complicated geometric domains the problem of creating meshes (or simply – meshing) is still a tricky question. Various meshless and meshfree approaches were developed to avoid spatial discretization. One of these methods is the so called *R-functions method (RFM)* which discretizes the underlying functional space.

In 1963 Kantorovich observed that the solution of the problem

$$-\Delta u(\mathbf{x}) = f(\mathbf{x}) \ \text{ in } \Omega, \quad u(\mathbf{x}) = 0 \ \text{ on } \partial\Omega,$$

where $\Omega \subset \mathbb{R}^k$, $u : \Omega \to \mathbb{R}$, $f : \Omega \to \mathbb{R}$, $\partial\Omega = \overline{\Omega} \setminus \Omega$ and $\mathbf{x} \in \Omega$, could be found in the form of product of two functions $u(\mathbf{x}) = \omega(\mathbf{x})\Phi(\mathbf{x})$, where the first one is used to **exactly** satisfy the boundary conditions and must possess the following properties:

$$\omega(\mathbf{x}) = 0 \ \text{ on } \partial\Omega, \quad \omega(\mathbf{x}) > 0 \ \text{ in } \Omega, \nabla\omega(\mathbf{x}) \neq 0 \ \text{ on } \partial\Omega,$$

and the second one, to satisfy the differential equation. Kantorovich also showed the solutions for some simple domains like circle and rectangle.

In 1964 Rvachev suggested a method how to build such a functions $\omega(\mathbf{x})$ for almost arbitrary domains with given properties. Thus, having the function $\omega(\mathbf{x})$ for a given domain, we can find $\Phi(\mathbf{x})$ either exactly or approximately in the form $\Phi(\mathbf{x}) \approx \sum_i^n C_i\phi_i(\mathbf{x})$, where $\phi_i(\mathbf{x})$ are known linearly independent basis functions which form a complete sequence in appropriate functional space, but should *not* satisfy the boundary conditions.

In this work the application of RFM to the solution of the Poisson equation with homogeneous Dirichlet boundary conditions in complicated 2D geometrical domain is shown. The convergence study includes the comparison of current results with standard finite element solution and the dependence of the number of coordinate functions on the relative error.

Authors would like to thank Prof. Lydia Kurpa, Prof. Andreas Griewank and Priv. Doz. Lutz Recke for helpful discussions.

IC/PP3163/013: Development of a 2D RBF image reconstruction toolbox for sharp edged images.

Presenter: Vincent Durante (University of Massachusetts, USA)
Co-author: Jae-Hun Jung (Univ. Massachusetts at Dartmouth, USA)

Radial basis functions are widely used for image reconstruction because of grid flexibility and the fast convergence of their approximations; in other words, the RBF methods are mesh-free and high order convergent. We will present the 2D image reconstruction based on radial basis function reconstruction for sharp edged images using a MATLAB toolbox as a GUI interface. Sharp edged images reconstructed using RBF interpolations, however, tend to yield Gibbs ringing effects on the images themselves.

To minimize Gibbs oscillations, the epsilon-adaptive method is employed in the developed GUI toolbox with which the shape parameter is adaptively chosen such that only the first order basis function is used near the neighborhood. To adopt this method, the functions called from the toolbox first detect the discontinuities in the image. The expansion coefficients and the concentration function derived from the first derivatives are used for the generation of an edge map. This edge map is defined where the product of the expansion coefficients and

the concentration functions yield high values.
We also use a domain splitting technique to develop the fast reconstruction algorithm. This technique is also used for the local image reconstruction near the discontinuity, which will be of the most interest to the user. We will present the RGB color image demonstrations using the toolbox. The non-uniform distribution in the reconstructed grid space and the Fourier filtering technique embedded in the toolbox will also be discussed.

02: Numerical Analysis, Minisymposia

IC/MP346/002: Model reduction: theory, methodology and software.

Organiser: Volker Mehrmann (TU Berlin, Germany)
Co-organiser: Zhaojun Bai (UC Davis, USA)
Co-organiser: Roland Freund (UC Davis, USA)

Model order reduction is currently one of the fundamental research areas in simulation and control of large-scale systems. Despite recent progress in the development of Krylov subspace methods, SVD-based methods, and POD methods, in most practical applications there is a discrepancy between fast and efficient methods to compute the reduced order model, preservation of physical properties of the system, like conservation laws, stability, passivity, or variational properties of the system.

There is a lot of research activity in this direction and it is the aim of this minisymposium to bring some of the key players in academia and industry together, to exchange the latest developments and to coordinate research activities. We focus on new and more efficient model reduction techniques, the theoretical foundations and new software developments.

Model reduction for robust control of large-scale systems. **Peter Benner** (TU Chemnitz, Germany) IC/MT1055/002

In this talk we consider the problem of robust control design for systems arising from the semi-discretization of parabolic evolution equations. Following the design methodology of H_∞ control, the usual two model reduction paths can be taken: reduce the plant, then design the controller or design a controller, then reduce it. In the first approach it is necessary to use model reduction techniques that guarantee the robust performance of the controller applied to the original system while for the second approach, it is desirable that the controller reduction preserves the performance (H_∞ norm bounds) of the controller. For these purposes, we will discuss techniques based on bounded-real and H_∞ balancing. We will demonstrate how they can be implemented for large-scale systems arising from finite differences or finite element disrectizations of parabolic control systems such as point and boundary control problems for the heat equation, convection-diffusion and reaction-diffusion equations.

Balancing-related model reduction by a data-sparse cross-Gramian approach. **Ulrike Baur** (TU Chemnitz, Germany), Peter Benner (TU Chemnitz, Germany) IC/MT1079/002

We consider linear time-invariant (LTI) systems of the following form:

$$\Sigma: \begin{cases} \dot{x}(t) &= Ax(t)+Bu(t), \qquad t>0, \qquad x(0)=x^0, \\ y(t) &= Cx(t)+Du(t), \qquad t\geq 0, \end{cases}$$

with stable state matrix $A \in R^{n\times n}$ and $B \in R^{n\times m}$, $C \in R^{p\times n}$, $D \in R^{p\times m}$, arising, e.g., from the discretization and linearization of parabolic PDEs. Typically, in practical applications, we have a large state-space dimension $n = \mathcal{O}(10^5)$ and a small input and output space, $n \gg m, p$. We further assume that the system is square; i.e., $p = m$.

We show how to compute an approximate reduced-order system $\hat{\Sigma}$ of order $r \ll n$ with a balancing-related model reduction method. The method is based on the computation of the cross-Gramian X, which is the solution of the Sylvester equation

$$AX + XA + BC = 0.$$

As standard algorithms for the solution of Sylvester equations are of limited use for large-scale systems, we investigate approaches based on the matrix sign function method. To make this iterative method applicable in the large-scale setting, we propose a modified iteration scheme for computing low-rank factors of the solution X and we incorporate structural information from the underlying PDE model into the approach. By using data-sparse matrix approximations, hierarchical matrix formats, and the corresponding formatted arithmetic we obtain an efficient solver having linear-polylogarithmic complexity. We show that the reduced-order model can then be computed from the low-rank factors directly.

Fast and stable solution of the Stein equation. **Ming Gu** (UC Berkeley, USA) IC/MT3603/002

We develop a fast and stable variant of the Hammarling Algorithm for solving the Stein equation in input-normal form. We present numerical experiments to confirm that it can be significantly faster than the Hammarling Algorithm.

Balanced truncation model reduction for the Oseen equations. **Danny Sorensen** (Rice University, USA), Matthias Heinkenschloss (Rice University, USA), Kai Sun (Rice University, USA) IC/MT4106/002

We discuss balanced truncation model reduction for the semidiscrete Oseen equations with time independent advection. These equations are related to linearized Navier-Stokes equations, so this model problem is relevant to many flow systems where the behavior of the linearized flow around a steady state is of interest. Balanced model reduction for linear time invariant systems is a scheme that preserves asymptotic stability and also provides an error bound on the discrepancy between outputs of the full and reduced order systems. The semidiscrete Oseen equations are a system of differential algebraic equations. Standard balanced truncation model reduction must be adapted to this descriptor system. The algorithm presented here offers a more direct approach than existing methods. In particular, no explicit projection operators are applied and a saddle point solver for Stokes-like linear systems is all that is required for implementation.

IC/MP346/002: Model reduction: theory, methodology and software. #2

Organiser: Volker Mehrmann (TU Berlin, Germany)
Co-organiser: Zhaojun Bai (UC Davis, USA)
Co-organiser: Roland Freund (UC Davis, USA)

(For abstract, see session #1 above.)

Model reduction from input/output measurements. **Athanasios Antoulas** (Rice University, USA) IC/MT4118/002

In many applications no explicit model of a given process is available. Instead input/output measurments of the process exist. The problem therefore consists in computing an appropriate approximate (reduced-order) model directly from these measurements. In this talk we will propose a method for achieving this objective. The main tool is the Loewner matrix. We will also show that this method can be extended to deal with passivity preserving model reduction. Numerical experiments verifying the theoretical considerations will also be provided.

A Krylov-based descent algorithm for optimal H^2 model reduction. **Serkan Gugercin** (Virginia Tech, USA), Christopher Beattie (Virginia Tech, USA) IC/MT4134/002

In this work, we introduce a Krylov-based descent algorithm for optimal H^2 approximation of large-scale dynamical systems where the interpolation points are the variables of the underlying optimization problem. After deriving the gradient and Hessian of the H^2 cost function with respect to interpolation points, a numerically effective optimal H^2 model reduction method is developed. Convergence properties and effectiveness of the algorithm are presented through numerical examples.

Interpolatory projection methods for structure-preserving model reduction. **Christopher Beattie** (Virginia Tech, USA), Serkan Gugercin (Virginia Tech, USA) IC/MT4186/002

We present a framework for interpolatory model reduction that includes rational Krylov-based methods as a special case. This broader framework allows retention of special structure in the reduced order models such as symmetry, second order structure, internal delays, and infinite dimensional subsystems. A rational strategy within this framework for the selection of interpolation points that produce near optimal $\mathcal{H}_\infty$ performance is also presented. Numerical examples are provided to illustrate and support the analysis.

How to solve realistic large-scale saddle-point problems. **Beresford Parlett** (University of California, Berkeley, USA), Jörg Liesen (TU Berlin, Germany) IC/MT4299/002

The coefficient matrix may be written $(AB'; B - C)$ in Matlab notation. A is symmetric positive definite, while C is only semidefinite. In some applications $C = O$. We give necessary and sufficient conditions to be able to solve the system with a CG iteration with a fancy, but economical, inner product. However in realistic applications these conditions are violated because $\|B\|$ is too big. We explore what happens when the inner product becomes indefinite and a look-ahead CG iteration copes with near breakdowns.

IC/MP181/015: Multiscale methods for strongly-heterogeneous media.

Organiser: Assyr Abdulle (University of Edinburgh, UK)

This minisymposium is concerned with the modeling and the numerical simulation of physical processes in strongly heterogeneous media as deformation or diffusion in heterogeneous material, flow in porous medium to mention but a few. A common aspect of these problems is that direct microscopic approaches resolving the heterogeneities of the media are often computationally intractable, due to the high number of degrees of freedom. Macroscopic approaches which do not take into account the fine scale physics are of limited interest, since the microscopic heterogeneities significantly affect the properties of the solution at all scales. There is a growing interest in computational techniques and simulation capable of extracting the effective macroscopic behavior of physical systems in heterogeneous media without resolving all the fine scale details. In this minisymposium key questions as adaptive modeling, efficient coupling of micro-to-macro methods, numerical control of hybrid methods, computational complexity of hierarchical numerical methods as well as some challenging applications will be discussed.

On local microscale problem in multiscale modeling. **Xingye Yue** (University of Science and Technology of China) IC/MT1807/015

Many multiscale methods for strongly heterogeneous media are based on the idea of extracting macroscopic information by solving an array of microscale models over small domains. A key ingredient in such multiscale methods is the boundary condition and the size of the computational domain over which the microscale problems are solved. We will discuss the effects of different boundary conditions and the local cell size for strongly heterogeneous media.

Heterogeneous multi-scale methods for epitaxial growth. **Björn Engquist** (University of Texas at Austin, USA) IC/MT3205/015

Continuum simulations of solids or fluids for which some atomistic information is needed are typical example of multiscale problems with wide ranges of scales. The heterogeneous multi-scale method is a framework for numerical methods that couple computations from very different scales. Local micro-scale simulations on small domains supply missing data to a macro-scale simulation on the full domain. In our example of epitaxial crystal growth, local kinetic Monte Carlo computations produce data to a continuum macro-scale level-set model for island growth.

Homogenization for mesocale oceanic transport and molecular motors. **Peter Kramer** (Rensselaer Polytechnic Institute, USA), Grigorios Pavliotis (Imperial College London, UK), Shafer Smith (New York University, USA), Juan Latorre (Rensselaer Polytechnic Institute, USA), Banu Baydil (Rensselaer Polytechnic Institute, USA) IC/MT3154/015

Two applications of the homogenization procedure will be presented. The first concerns the parameterization of the effects of mesoscale coherent structures on the transport of physical fields in the ocean. We are developing our parameterization procedure from the bottom up, beginning with rather simple mathematical models and combining them with numerical solutions of the cell problems and asymptotic analysis with respect to physical parameters such as Peclet number, Strouhal number, and relative mean flow strength in an attempt to achieve an efficient scheme for relating the large-scale transport to the physical properties of the subgrid structures. At present, the velocity field is treated kinematically.

The second application concerns the use of the homogenization theory to compute transport properties of molecular motors, which we treat within the mathematical framework of "Brownian motors." We examine in particular, through numerical computation and asymptotic analysis, how the effective drift as well as the coherence of transport (as represented by a

Peclet number) behave with respect to the underlying physical parameters of the forces and motor driving time scales. We are also particularly concerned with efficient numerical means of solving the equations produced by the cell problems.

IC/MP181/015: Multiscale methods for strongly-heterogeneous media. #2

Organiser: Assyr Abdulle (University of Edinburgh, UK)

(For abstract, see session #1 above.)

Sparse adaptive FEM for multiple-scale problems. **Christoph Schwab** (ETH Zürich, Switzerland) IC/MT1910/015

Elliptic homogenization problems in a domain $\Omega \subset R^d$ with $n+1$ separated scales are reduced to elliptic one-scale problems in dimension $(n+1)d$ using multiscale convergence techniques of G. Allaire and M. Briane. The $(n+1)d$ dimensional, one-scale limit problems are discretized by a sparse tensor product finite element method (FEM) in the physical domain and all 'cells'. We prove that the resulting FEM has accuracy, work and memory requirement comparable to standard FEM for single scale problems in Ω while it gives numerical approximations of the correct homogenized limit as well as of all first order correctors, throughout the physical domain with performance independent of the physical problem's scale parameters and the full approximation order in terms of the number N of degrees of freedom in the physical domain Ω.

Condition numbers of the discrete problems are bounded uniformly in the number of scales as well as in the scale parameters.

Joint work w. V. H. Hoang (Cambridge) and R. Stevenson (Utrecht).

An analytical framework for the numerical homogenization of integral functionals. **Antoine Gloria** (Ecole Nationale des Ponts et Chaussées, France) IC/MT1553/015

We present one possible analytical framework to clarify some convergence properties of numerical homogenization schemes to deal with heterogeneous media. This approach completes previous results existing in the literature. The problem under consideration is the minimization of a nonlinear integral functional, both in the convex and quasiconvex settings, with and without spatial assumptions such as periodicity or stochasticity. This approach relies on variational calculus and Γ-convergence. It allows to address some aspects of nonlinear elasticity such as the frame invariance property. We also address the issue of convergence of the numerical correctors for monotone elliptic operators without assumption on the structure of the heterogeneities, and we provide some new error estimates in the periodic case.

Analysis of multiscale methods: methodology and examples. **Pingbing Ming** (Chinese Academy of Sciences), Pingwen Zhang (Peking University, PR China), Xingye Yue (University of Science and Technology of China) IC/MT2060/015

Analysis of multiscale methods presents a challenge to numerical analyst, particularly for problems involving multi-physics. The heterogeneous multiscale method gives a general framework for the analysis of multiscale methods besides providing guidelines for the design of the method. In this talk, I will demonstrate this by applying the framework to two canonical problems: partial differential equations with multiscale coefficients as well as the local quasicontinuum methods.

This is a joint work with Weinan E (PACM, Princeton University), Pingwen Zhang (University of Beijing) and Xingye Yue (University of Science and Technology).

Finite-element heterogeneous multiscale methods with near-optimal computational complexity. **Assyr Abdulle** (University of Edinburgh, UK), Björn Engquist (University of Texas at Austin, USA) IC/MT2752/015

Macro-to-micro numerical methods have become increasingly popular for the multiscale modelling of problems often impossible to solve by direct numerical simulations.

In this talk we discuss macro-to-micro finite element methods constructed in the framework of the heterogeneous multiscale method (HMM). The global behaviour of such methods depends on the hierarchy of solvers and on the strategy to couple them. A fully discrete analysis is crucial for the understanding of error propagation across scales and the global complexity is in general superlinear in the macro degrees of freedom. In this talk we discuss how to couple macro methods with fast micro solvers in order to achieve near optimal computational complexity for finite element heterogeneous multiscale methods.

References.

[1] A. Abdulle and B. Engquist : Finite element heterogeneous multiscale methods with near optimal computational complexity, submitted to SIAM MMS.

[2] A. Abdulle : On a-priori error analysis of fully discrete heterogeneous multiscale FEM, SIAM MMS, Vol. 4, No 2, 2005.

IC/MP802/015: Verified computations with applications.

Organiser: Siegfried Rump (TU Hamburg-Harburg, Germany)
Co-organiser: Shinichi Oishi (Waseda University, Japan)

Recently, the research in the field of verified numerical computations has made great progress. This minisymposium focuses on recent advances and gathers 8 papers from 5 countries, namely Japan, three countries in Europe and USA.

Starting from the presentation of recent results on highly accurate and fast summation algorithms, presentations for algorithms for numerical verification of geometric predicates and fast and accurate polynomial evaluation based on these summation algorithms will follow. Then, constraint global optimization with verification of the result will be discussed within a general framework of computer assisted proofs. As concrete examples of computer assisted proofs, scattering problems of sound and light, numerical existence and uniqueness theorems for PDEs and bifurcation problems will be treated. Finally, relations and applications to fuzzy logic will also be discussed.

This variety of talks will elucidate the state of arts of the rapidly developing research field on verified numerical computations.

Error bounds for extremely ill-conditioned problems. **Siegfried Rump** (TU Hamburg-Harburg, Germany) IC/MT2960/015

We discuss methods to compute error bounds for extremely ill-conditioned problems. As a model problem we treat matrix inversion. We demonstrate that additive corrections to improve an approximate inverse are useful for ill-conditioned problems, but hardly usable for extremely ill-conditioned problems. Here multiplicative corrections can be used, including the possibility to compute guaranteed error bounds. Problem with condition numbers 1e100 and more are solved in double precision.

Fast and accurate floating-point summation. **Takeshi Ogita** (Japan Science and Technology Agency), Siegfried Rump (TU Hamburg–Harburg, Germany), Shinichi Oishi (Waseda University, Japan) IC/MT2799/015

Recently, we proposed a new accurate summation algorithm. For a floating-point vector p, the algorithm returns a result faithfully rounded from the exact summation of p. Moreover, it is very fast in terms of not only flop counts but also measured computing time. In this talk, we try to make the algorithm speed up further. For the purpose, we use a grouping of the elements in p without any sorting. The summation algorithm with our speedup method is faster than or at worst equal to the original one. The speedup method does not change any analysis for the summation algorithm, i.e. it returns exactly the same (faithful) result as that from the original one. The effectiveness of the speedup method strongly depends on how the data of various magnitude are distributed in p.

First in the talk, we briefly review our new accurate summation algorithm. Next, we explain how to speedup the algorithm. Finally, numerical results are presented showing performance of the proposed speedup method.

Faithful Horner algorithm. **Philippe Langlois** (Université de Perpignan, France), Nicolas Louvet (Université de Perpignan, France) IC/MT3342/015

Compensated Horner algorithm consists in correcting the rounding errors generated by floating point computation of the classic Horner algorithm for polynomial evaluation. Using what Rump, Ogita and Oishi named error free transformations in [1], the compensated Horner algorithm is proved to be as accurate as the Horner algorithm computed with twice the current precision. Iterating such correction we also provide another compensated Horner algorithm proved to be as accurate as the Horner algorithm performed in k times the working precision. These compensated algorithms are fast and compare favorably with double-double or quad-double corresponding implementations. We will present new results about this compensated Horner algorithm that allow us to efficiently compute a *faithful polynomial evaluation*, that is to return one of the two nearest floating point numbers that enclose the exact polynomial evaluation. [1] Ogita, T., Rump S.M. and Oishi S.; *Accurate sum and dot product*, SIAM J. Sci. Comput., 26(6):1955:1988, 2005.

Fast and adaptive algorithm for 2D orientation problem. **Katsuhisa Ozaki** (Waseda University, Japan), Takeshi Ogita (Japan Science and Technology Agency), Siegfried Rump (TU Hamburg–Harburg, Germany), Shinichi Oishi (Waseda University, Japan) IC/MT4951/015

This talk is concerned with the computational geometry. A number of geometric problems can be boiled down to the determinant predicates, i.e. whether the sign of the determinant is positive, negative or zero. In particular, we focus our mind on the 2D orientation problem ORIENT2D, which determines whether a point is exactly on a line or on which side it is in two dimensional space. If the point is close to the line, one may obtain an incorrect result due to rounding errors by usual floating-point computations. To solve such ill-conditioned cases, some higher precision is necessary. On the other hand, it is not efficient to use higher precision arithmetic for well-conditioned cases.

In this talk, we propose a fast, robust and adaptive algorithm of solving ORIENT2D based on a new accurate summation algorithm which is developed by the latter three authors (S. M. Rump, T. Ogita and S. Oishi). If given points are represented by floating-point numbers, the computation of determinant can be transformed into a computation of summation without rounding errors. Since their algorithm can verify an accuracy of the obtained result, the sign of the determinant can also be guaranteed. By specializing their algorithm for the computation of the determinant with considering the structure of data for floating-point summation and devising a way of its implementation, computational cost for solving ORIENT2D can efficiently be reduced. Moreover, to make an adaptive algorithm is also possible, i.e. its computational cost increases gradually according to the difficulty of a given problem.

Finally, some numerical results are presented showing that our proposed algorithm is faster than the state-of-the-art one by Shewchuk's one in many cases.

IC/MP802/015: Verified computations with applications. #2

Organiser: Siegfried Rump (TU Hamburg–Harburg, Germany)
Co-organiser: Shinichi Oishi (Waseda University, Japan)

(For abstract, see session #1 above.)

Verified global optimization with GloptLab. **Ferenc Domes** (Universität Wien, Austria), Arnold Neumaier (Universität Wien, Austria) IC/MT3426/015

We present GloptLab, a MATLAB toolbox for the verified global optimization of quadratic functions with quadratic constraints. The main tools used are local optimization, semidefinite programming, branch and bound, interval analysis and constraint programming. Powerful new techniques allow many problems to be solved with a comparatively small branch tree. For potential applications to computer-assisted proof, some emphasis is given to generate a list of certificates that enables a simple proof checker to verify the validity of the global optimum with mathematical rigor, and a human readable version of the proof outline, with links to more details as far as desired.

On constructive a priori *and* a posteriori *error estimates for the finite-element approximations of non-coercive elliptic problems.* **Mitsuhiro Nakao** (Kyushu University, Japan), Kouji Hashimoto (Kyoto University, Japan) IC/MT2100/015

On the finite element method for noncoercive linear elliptic boundary value problems, there are no existing techniques to get *a priori* and/or *a posteriori* error estimates. For such kind of problems, we have to know the invertibility of concerning elliptic operators. In this talk, by using the invertibility condition which was established by the authors, we present a method enabling us to determine the actual constant appearing in the *a priori* error etimates even for noncoercive case. We also give an efficient method to obtain *a posteriori* error estimates for the same problem. These results can also be applied to the *a posteriori* error estimates for solutions of nonlinear elliptic problems. Several numerical examples which confirm the actual usefulness of the method will be presented.

Enclosure methods and computer-assisted proofs for nonlinear elliptic boundary value problems. **Michael Plum** (Universität Karlsruhe, Germany) IC/MT3226/015

The lecture will be concerned with numerical enclosure methods for nonlinear elliptic boundary value problems. Here, analytical and numerical methods are combined to prove rigorously the existence of a solution in some "close" neighborhood of an approximate solution computed by numerical means. Thus, besides the existence proof, verified bounds for the error (i.e. the difference between exact and approximate solution) are provided.

For the first step, consisting of the computation of an approximate solution ω in some appropriate Sobolev space, no error control is needed, so a wide range of well-established numerical methods (including multigrid schemes) is at hand here. Using ω, the given problem is rewritten as a *fixed-point equation* for the error, and the goal is to apply a *fixed-point theorem* providing the desired error bound.

The conditions required by the chosen fixed-point theorem (e.g., compactness or contractivity, inclusion properties for a suitable subset etc.) are now verified by a combination of analytical arguments (e.g. explicit Sobolev embeddings, variational characterizations etc.) and verified computations of certain auxiliary terms, in particular of eigenvalue bounds for the linearization of the given problem at ω.

The method is illustrated by several examples (on bounded as well as on unbounded domains), where in particular it gives existence proofs in cases where no purely analytical proof is known.

Numerical uniqueness and existence theorem for solution of Lippmann–Schwinger equation to 2D sound-scattering problem. **Shinichi Oishi** (Waseda University, Japan) IC/MT2792/015

In this paper, we are concerned with a scattering problem for the Helmholtz equation in the inhomogeneous media. It is well known that this problem is given as a mathematical modeling of a two dimensional sound scattering problem.

In this talk, for the sake of simplicity, we treat the case that the problem have a smoothness $W^{\mu,2}(\mathbb{R}^2)$, $\mu \geqq 3/2$ and present Theorem giving a sufficient condition of guaranteeing that the homogeneous equation corresponding to the original equaiton has in H^0 only the trivial solution. A remarkable feature of this theorem is that the sufficient condition shown in this theorem can be evaluated by verified numerical computations. Furthermore, if such a sufficient condition holds, it also gives an upper bound of $\|(I - aK)^{-1}\|_{\mathcal{L}(H^0)}$ and a tight error bound between the exact solution v and an approximate solution $\tilde{v}$ which is generated by computer. As a result, this paper is to present a numerical uniqueness and existence theorem for the problem, which asserts the existence of a unique solution around an approximate solution computed by numerical calculation.

IC/MP333/020: Large-scale eigenvalue problems.

Organiser: Peter Arbenz (ETH Zürich, Switzerland)

Recent years have seen the emergence of a number of new algorithms for the solution of large scale eigenvalue problems. Large scale eigenvalue problems are so big that the involved matrices can not be factored such that a standard shift-and-invert Lanczos algorithm is not a suitable solution method. The speakers of this minisymposium will discuss ways to overcome this problem presenting Arnoldi-/Lanczos-like, versions of Davidson/Jacobi–Davidson and Locally Optimal Block Preconditioned Conjugate Gradient (LOBPCG) Algorithm to solve large eigenvalue problems from science and engineering.

Enhancements to the PRIMME eigenvalue package and recent experimental results. **Andreas Stathopoulos** (College of William and Mary, USA) IC/MT2033/020

PRIMME, or PReconditioned Iterative MultiMethod Eigensolver, is a comprehensive, open source software package for solving large, sparse, Hermitian eigenvalue problems. While implementing advanced, near optimally converging methods, it has a very simple interface that requires little, or no parameter tuning. Moreover, our new DYNAMIC algorithm, alternates between methods to find the best at runtime. We review this and other PRIMME enhancements, and present experimental results from a variety of application areas that demonstrate PRIMME's superior robustness and efficiency over other state-of-the-art eigenvalue software.

*Block locally-optimal pre-conditioned eigenvalue xolvers (*BLOPEX*).* **Andrew Knyazev** (University of Colorado at Denver, USA) IC/MT3644/020

Block Locally-Optimal Preconditioned Eigenvalue Xolvers (BLOPEX) is a package, written in C, that at present includes only one eigenxolver, Locally Optimal Block Preconditioned Conjugate Gradient Method (LOBPCG). BLOPEX supports parallel computations through an abstract layer. BLOPEX is incorporated in the HYPRE package from LLNL and is availabe as an external block to the PETSc package from ANL as well as a stand-alone serial library. Hypre and PETSc packages provide high quality multigrid and domain decomposition preconditioning on parallel clusters with distributed or shared memory architecture.

The LOBPCG method, suggested and developed by Andrew Knyazev [1] in the past decade, recently attracts an increasing attention as a potential alternative to the shift-and-invert Lanczos and preconditioned Davidson methods due to its simplicity, robustness and fast convergence. Several MATLAB, C, C++ and FORTRAN implementations of the LOBPCG are developed by different groups, e. g., for such applications areas as structured mechanics and electronic structure calculations.

Main LOBPCG features: a matrix-free iterative method for computing several extreme eigenpairs of symmetric positive generalized eigenproblems; a user-defined preconditioner; robustness with respect to random initial approximations, variable preconditioners, and ill-conditioning of the stiffness matrix; apparently optimal convergence speed.

We present initial scalability results using BLOPEX with Hypre and PETSc on one BlueGene/L box solving eigenvalue problems of record sizes.

[1] A.V. Knyazev, "Toward the Optimal Preconditioned Eigensolver: Locally Optimal Block Preconditioned Conjugate Gradient Method." SIAM Journal on Scientific Computing 23 (2001), no. 2, pp.517–541.

Robust expansion of subspaces in iterative projection methods. **Heinrich Voss** (TU Hamburg–Harburg, Germany) IC/MT1064/020

Iterative projection methods for large eigenproblems have proven to be very efficient if a small number of eigenvalues and eigenvectors are desired. Here the eigenproblem is projected to a subspace of small dimension which yields approximate eigenpairs. If an error tolerance is not met then the search space is expanded in an iterative way with the aim that some of the eigenvalues of the reduced matrix become good approximations of some of the wanted eigenvalues of the given large matrix.

Expanding the subspace by the Jacobi-Davidson method is very efficient. It is known to converge at least quadratically if the correction equation is solved exactly, and it is common experience that the fast convergence is maintained if the correction equation is solved only approximately. In this talk we derive the Jacobi–Davidson method in a way that explains this robust behavior.

Iterative computation of band edge states for semi-conductor nano structures. **Christof Voemel** (Lawrence Berkeley National Laboratory, USA) IC/MT2591/010

The so-called band edge states determine optical and electronical properties of semi-conductor nano structures. They can be computed from an interior eigen-problem. We study the robustness and performance of state-of-the-art iterative eigensolvers on large quantum dots and wires, focusing on variants of preconditioned CG, Lanczos, and Davidson methods.

IC/MP333/020: Large-scale eigenvalue problems. #2

Organiser: Peter Arbenz (ETH Zürich, Switzerland)

(For abstract, see session #1 above.)

A Jacobi–Davidson algorithm for large eigenvalue problems from opto-electronics. **Peter Arbenz** (ETH Zürich, Switzerland) IC/MT3641/020

The construction of prototypes of nowadays opto-electronic components during their development is very expensive. Therefore, they are developed and simulated on the computer. This procedure admits to determine and optimize their characteristics, in particular their optical characteristics, in advance. The progressive miniaturization of opto-electronic components leads to numerous quantum-mechanical effects, that cannot be treated by the usual classical models. Quantum-mechanical methods have to be employed. The states of the charge carriers and the dispersion relations are determined by coupled Schrödinger equations. Their discretization by means of the finite element method leads to large sparse generalized complex Hermitian eigenvalue problems. Because of their size the solution of these eigenvalue problems requires sophisticated eigensolvers. We present a variant of the Jacobi–Davidson (JD) algorithm that is based on a real symmetric formulation of the complex Hermitian eigenvalue problem. The correction equations that have to be solved in each step of JD are solved by the conjugate gradient algorithm preconditioned by a V-cycle of smoothed aggregation multigrid.

On large-scale diagonalization techniques for the Anderson model of localization. **Olaf Schenk** (Universität Basel, Switzerland), Matthias Bollhöfer (TU Braunschweig, Germany) IC/MT1227/020

We propose efficient preconditioning algorithms for an eigenvalue problem arising in quantum physics, namely the computation of a few interior eigenvalues and their associated eigenvectors for large-scale sparse real and symmetric indefinite matrices of the Anderson model of localization. We compare the Lanczos algorithm in the 1987 implementation by Cullum and Willoughby with the shift-and-invert techniques in the implicitly restarted Lanczos method and in the Jacobi–Davidson method. Our preconditioning approaches for the shift-and-invert symmetric indefinite linear system are based on maximum weighted matchings [1] and algebraic multilevel incomplete LDL^T factorizations. These techniques can be seen as a complement to the alternative idea of using more complete pivoting techniques for the highly ill-conditioned symmetric indefinite Anderson matrices. We demonstrate the effectiveness and the numerical accuracy of these algorithms. Our numerical examples reveal that recent algebraic multilevel preconditioning solvers can accelerate the computation of a large-scale eigenvalue problem corresponding to the Anderson model of localization by several orders of magnitude[2].

This is joint work with Matthias Bollhöfer (TU Brunswick) and Rudolf Römer (University of Warwick).

[1] Hagemann, M. and Schenk, O.; Weighted matchings for the preconditioning of symmetric indefinite linear systems. SIAM Journal of Scientific Computing, 28 (2006), pp.403–420.

[2] Schenk, O., Bollhöfer, M. and Römer, R.; On large-scale diagonalization techniques for the Anderson model of localization. SIAM Journal of Scientific Computing, 28 (2006), pp.963–983.

Polynomial-filtered Lanczos iterations with applications in electronic-structure calculations. **Konstantinos Bekas** (IBM Zurich Research Laboratory, Switzerland), Yousef Saad (University of Minnesota, USA) IC/MT1445/020

The most expensive part of all Electronic Structure Calculations based on Density Functional Theory, lies in the computation of an invariant subspace associated with some of the smallest eigenvalues of a discretized Hamiltonian operator. The dimension of this subspace typically depends on the total number of valence electrons in the system, and can easily reach hundreds or even thousands when large systems with many atoms are considered. At the same time, the discretization of Hamiltonians associated with large systems yields very large matrices, whether with plane-wave or real space discretizations. The combination of these two factors results in one of the most significant bottlenecks in Computational Materials Science. In this paper we show how to efficiently compute a large invariant subspace associated with the smallest eigenvalues of a symmetric/hermitian matrix using polynomially filtered Lanczos iterations. The proposed method does not try to extract individual eigenvalues and eigenvectors. Instead, it constructs an orthogonal basis of the invariant subspace by combining two main ingredients. The first is a filtering technique to dampen the undesirable contribution of the largest eigenvalues at each matrix-vector product in the Lanczos algorithm. This technique employs a well-selected low-pass filter polynomial, obtained via a conjugate residual-type algorithm in polynomial space. The second ingredient is the Lanczos algorithm with partial reorthogonalization. Experiments are reported to illustrate the efficiency of the proposed scheme compared to state-of-the-art implicitly restarted techniques.

Solving large-scale nonlinear eigenvalue problems in electronic-structure calculation. **Chao Yang** (Lawrence Berkeley National Laboratory, USA) IC/MT3108/020

One of the fundamental problems in electronic structure calculation is to determine electron orbitals associated with the minimum total energy of large atomistic systems. The total energy minimization problem is often formulated as a nonlinear eigenvalue problem and solved by an iterative scheme called Self Consistent Field (SCF) iteration. In this talk, a new direct constrained optimization algorithm for minimizing the Kohn-Sham (KS) total energy functional is presented. The key ingredients of this algorithm involve projecting the total energy functional into a sequences of subspaces of small dimensions and seeking the minimizer of total energy functional within each subspace. The minimizer of the projected energy functional not only provides a search direction along which the KS total energy functional decreases but also gives an optimal "step-length" to move along this search direction. Due to the small dimension of the projected problem, the minimizer of the projected energy functional can be computed by several different methods. These methods will be examined and compared in this talk. Numerical examples will be provided to demonstrate that this new direct constrained optimization algorithm can be more efficient and robust than the SCF iteration.

IC/MP277/020: Tensor decompositions and their application.

Organiser: Brett Bader (Sandia National Laboratories, USA)
Co-organiser: Tamara Kolda (Sandia National Laboratories, USA)

Tensors, also known as multidimensional, multi-way, or n-way arrays, are higher-order analogues of matrices. The Tucker and CANDECOMP/PARAFAC (CP) tensor decompositions were introduced more than three decades ago in the context of psychometrics and can be thought of as generalizations of the matrix singular value decomposition (SVD). The Tucker and CP tensor decompositions have since proven useful in a variety of fields including chemometrics, signal processing, computer graphics, statistics, etc. Using multilinear algebra rather than standard linear algebra has the advantage of yielding, in many cases, smaller and more meaningful factorizations. Moreover, it may not be necessary to impose orthogonality to yield uniqueness.

The Tucker and CP tensor decompositions are closely related to methods that exploit Kronecker or Khatri–Rao product structure in matrices. In this session, the speakers will present extensions of the Tucker and CP tensor decompositions to nonnegative and block (i.e., a combination of Tucker and CP) tensor factorizations. Additionally, the session will highlight algorithmic and computational aspects of handling large-scale, sparse, noisy, and/or missing data for applications in chemistry, medicine, network analysis, and data mining. The first presentation will provide an overview of tensor decompositions and their relevance.

The decomposition in rank-$(L, L, 1)$ terms: an approach based on simultaneous matrix diagonalization. **Lieven De Lathauwer** (CNRS-ETIS, France) IC/MT1879/012

The Canonical decomposition or Parallel factor decomposition (CP) in multilinear algebra is the decomposition of a higher-order tensor in a sum of rank-1 terms. Contrary to the Singular Value Decomposition of matrices, CP is unique without imposing orthogonality conditions on the factors. Uniqueness is guaranteed under the so-called 'Kruskal condition'.

Recently we have considered the case of 'long' tensors, i.e., tensors of which one of the dimensions is greater than the rank. For such tensors, we have derived a uniqueness condition that is much more relaxed than Kruskal's. The proof of the theorem is constructive. It shows that, for exact data, CP follows from the Eigenvalue Decomposition (EVD) of a matrix. For noisy data we have proposed an algorithm based on a simultaneous matrix decomposition.

Recently, we have also proposed a generalization of CP in which each term consists of the outer product of a vector and a rank-L matrix, L being relatively small but greater than one. Uniqueness is guaranteed under Kruskal-type conditions.

In this talk we will combine the two new ideas. That is : (1) we will show that, in the case of exact data, the decomposition in rank-(L,L,1) terms of a long tensor follows from a matrix EVD, (2) for noisy data, we will propose an algorithm based on a simultaneous matrix decomposition, (3) we will present new sufficient conditions for uniqueness that are significantly more relaxed than the Kruskal-type conditions.

Blind source separation and automatic transcription of music using tensor decompositions. **Derry FitzGerald** (Cork Institute of Technology, Ireland) IC/MT416/012

Tensor decompositions have recently found use in the sound source separation and automatic transcription of musical recordings. The majority of musical recordings available are stereo recordings created by linear mixing of single channel recordings of different instruments, with different gains in each channel to create a stereo image. Non-negative tensor decomposition is carried out on a tensor containing magnitude spectrograms of each channel of the input signals, yielding sets of basis functions corresponding to aspects of the musical recording, such as a note played by a musical instrument. These basis functions can then be grouped together by source, allowing the creation of a magnitude spectrogram containing information related to a single sound source. Grouping of the basis functions can be done using a variety of criteria, such as statistical dependencies between basis functions, or grouping by similar gain patterns across the channels. However, in many cases, it is difficult to automatically assign the basis functions to sources.

This grouping problem can be overcome by incorporating frequency shift invariance into the tensor decomposition model. This allows notes played by an instrument to be modeled as translations of a single instrument basis function, thereby eliminating the need to cluster the basis functions. Further, as the timbre of musical instruments evolve with time, a single basis function cannot capture this time evolution. This can be modeled by adding time shift invariance to the model, resulting in a musical instrument being modeled as a spectrogram that is translated in frequency to correspond to different notes played by the instrument. A transcription of the notes played by a given instrument can then be obtained from the activations of each translation of that instrument. This demonstrates the utility of a tensor decomposition approach, in that both sound source separation and automatic transcription are obtained simultaneously.

Tensor decompositions in chemistry. **Giorgio Tomasi** (Københavns Universitet, Denmark) IC/MT2759/012

Nowadays, many common analytical instruments and chemical problems generate $N-$way data arrays (for $N > 2$) whose systematic part is well described by so-called multilinear models; for this reason such models are growing increasingly popular in chemometrics. This presentation will focus on three of them: the PARAFAC (from 'PARAllel FACtors') model, which is essentially a best low-rank approximation of the data tensor; the $N-$way Tucker model, which is akin to the Singular Value Decomposition for matrices, and, for regression problems, the nPLS model, which is an extension of Partial Least Squares regression.

The use of such models on chemical data will be illustrated by means of practical examples together with some details on the state of the art on fitting algorithms and on open theoretical and practical challenges associated with them.

The Matlab tensor toolbox for efficient computations with sparse and factored tensors. **Tamara Kolda** (Sandia National Laboratories, USA), Brett Bader (Sandia National Laboratories, USA) IC/MT1478/012

This talk considers tensors with special structure and how their structure might be exploited for efficient storage and computation. Sparse tensors have the property that the vast majority of the elements are zero. We propose storing such tensors using coordinate format and consider the computational efficiency of this scheme for mathematical operations typical of those used in tensor decomposition algorithms. Factored tensors have the property that they can be assembled from components. We consider two specific types: a Tucker tensor can be expressed as the product of a core tensor (which itself may be dense, sparse, or decomposed) and a matrix along each mode, and a Kruskal tensor can be expressed as the sum of rank-1 tensors. We are interested in the case where the storage of the components is less than the storage of the full tensor and demonstrate that many elementary operations can be computed using only the components. All of the efficiencies described in this talk are implemented in the Tensor Toolbox for MATLAB.

IC/MP277/020: Tensor decompositions and their application. #2

Organiser: Brett Bader (Sandia National Laboratories, USA)
Co-organiser: Tamara Kolda (Sandia National Laboratories, USA)

(For abstract, see session #1 above.)

An overview of tensor decompositions and their applications. **Brett Bader** (Sandia National Laboratories, USA) IC/MT404/012

This presentation will introduce recent decompositions and applications of tensors (also known as multidimensional, multiway, or n-way arrays). Higher-order tensor decompositions originated in the field of psychometrics more than thirty years ago and have since become a promising technique in chemometrics, image analysis, signal processing, and, more recently, data mining. Researchers from a number of fields have applied tensor decompositions to some exciting applications with convincing results.

By incorporating extra information in higher-order data arrays, tensor decompositions are capable of extracting structure beyond traditional matrix analysis, such as the singular value decomposition (SVD) or principal components analysis (PCA). PARAFAC and the Tucker model are just two tensor decompositions for extracting information for some applications, but even more decompositions exist or are being proposed. Many challenges exist in deriving and applying these decompositions, including determining the proper model for the application, determining the appropriate rank of the approximation, and making any algorithms computationally efficient. As these techniques are applied to ever larger problems, another challenge is to find ways to extend these methods to large-scale data sets, i.e., data sets with thousands to millions of entries. This will require advances in the theory and computation of higher-order tensor decompositions.

This presentation first will introduce the mathematics and algorithms of tensor decompositions from an applied mathematics perspective and, second, will survey some applications across a variety of disciplines.

Sparseness constraints and non-negative tensor decomposition. **Morten Mørup** (Danmarks Tekniske Universitet, Denmark) IC/MT741/012

Higher order matrix (tensor) decompositions are mainly used in psychometrics, chemometrics, image analysis, graph analysis and signal processing. For higher order data the two most commonly used decompositions are the PARAFAC and the TUCKER model. If the data analyzed is non-negative it may be relevant to consider additive non-negative components. Non-negative matrix factorization (NMF) can easily be extended to form algorithms for non-negative TUCKER and PARAFAC decompositions. Furthermore, the PARAFAC model can be extended to account for shift and echo effects in the data by extending concepts from matrix deconvolution to tensors. To improve the uniqueness of the decomposition constraints in the form of the L1 norm is useful. Several algorithms are devised for non-negative decomposition of multi-way data (tensors) and their performance demonstrated on a range of datasets spanning from neuroscience and chemometry to music signals.

Computing the best rank-(R_1, R_2, R_3) approximation of a tensor. **Lars Eldén** (Linköpings universitet, Sweden) IC/MT535/012

We investigate various properties of the best rank-(R_1, R_2, R_3) approximation of a tensor, and their implications in the development of algorithms for computing the approximation. Often alternating methods are used for computing the solution of this problem. We investigate the convergence properties of alternating iteration and present alternative methods with faster convergence, including the variable projection and Newton-Grassmann method.

This is joint work with Berkant Savas.

Understanding epilepsy seizure structure using tensor decompositions. **Evrim Acar** (Rensselaer Polytechnic Institute, USA) IC/MT428/012

Epilepsy surgery outcome strongly depends on the localization of epileptic focus. We address the problem of identification of seizure origin through an analysis of ictal EEG, which is proven to be an effective standard in epileptic focus localization.

With a goal of presenting an automated and robust way of visual analysis of large amounts of EEG data, we construct a multiway EEG data array with three modes, i.e. time samples, scales and electrodes, through wavelet transformation. We then study the performance of multiway analysis techniques, particularly Parallel Factor Analysis (PARAFAC), in understanding the complex structure of epilepsy seizure and localization of seizure origin.

Our preliminary results on patients with temporal lobe epilepsy reveal that multiway analysis techniques are capable of capturing epileptic focus precisely when validated with clinical findings.

IC/MP255/020: Computational methods for structured eigenvalue problems.

Organiser: Peter Benner (TU Chemnitz, Germany)
Co-organiser: Daniel Kressner (Umea University, Sweden)

Linear and nonlinear eigenvalue problems that arise from applications in engineering, chemistry or physics are typically highly structured. Classes of structured matrices that have traditionally been a central issue in numerical linear algebra are symmetric, Hermitian, sparse, Toeplitz, Hankel, Hamiltonian and symplectic matrices, the latter two being related also to the solution of algebraic Riccati equations. Apart from those, new structures have emerged in recent years. These are often connected to linearizations of quadratic or rational eigenproblems. The associated matrix pencils are called even, odd, or palindromic. Currently, the development of numerical algorithms for these new matrix pencil structures is making rapid progress. In many cases, the matrix representations are not only highly redundant but also reflect some physical properties from the original problem. Consequently, the exploitation of these structures can have significant positive effects on the efficiency and accuracy of computational methods and therefore lies at the heart of modern numerical linear algebra. This minisymposium covers several aspects of structured eigenvalue problems, with emphasis on reliable and effective numerical methods.

HAPACK: software for structured eigenvalue problems. **Daniel Kressner** (Umea University, Sweden), Peter Benner (TU Chemnitz, Germany) IC/MT1476/020

HAPACK is a software package containing Fortran and Matlab routines for solving structured eigenvalue problems. This talk introduces version 2.0 of HAPACK extending its functionality significantly. A number of new routines address the computation of eigenvalues and invariant subspaces of matrix products in a numerically backward stable manner. This also allows to cover several classes of generalized eigenvalue problems, including (skew-)Hamiltonian, (skew-)symmetric, and symplectic pencils. For some of these classes, structure-preserving variants of Krylov subspace methods are implemented, providing functionality for large and sparse eigenvalue problems. The aim of this talk is to illustrate the use of HAPACK for practical applications and its benefits compared to general-purpose eigenvalue solvers, as, e.g., implemented in Matlab's eig and eigs commands. This is joint work with other contributors to HAPACK.

Computing the SVD of symplectic matrices. **Niloufer Mackey** (Western Michigan University, USA) IC/MT2825/020

It has recently been shown that every symplectic matrix has a *symplectic SVD*; i.e., an SVD in the usual sense in which each factor is also symplectic. We present a structure-preserving one-sided Jacobi algorithm to compute the symplectic SVD of any $2n \times 2n$ matrix. The method uses at most n^2 iterations per sweep, introducing zeroes via sorting symplectic orthogonal transformations that can be efficiently computed at each iteration. The algorithm is parallelizable, and the convergence rate is asymptotically quadratic.

This is joint work with A. Chaiyakarn.

Sort-Jacobi and generalizations of the symmetric-eigenvalue problem. **Martin Kleinsteuber** (Universität Würzburg, Germany) IC/MT1146/020

In the first part of the talk it is shown how several well-known structured eigenvalue and singular-value problems can be considered as a Lie algebraic generalization of the symmetric eigenvalue problem (EVP). Due to the well known classification of semi-simple Lie algebras, these include the real and complex SVD, hermitian and skew-Hermitian Hamiltonian EVP, the skew-symmetric EVP and Takagi's factorization as well as a Takagi-like factorization and three other interesting non-equivalent EVPs.

In the second part, a structure preserving Sort-Jacobi algorithm is presented to solve the above mentioned structured EVP/SVDs. The proposed method applies to an arbitrary semisimple Lie algebra on its (-1)-eigenspace of the Cartan involution. The proof of local quadratic convergence is sketched.

Structure-preserving doubling algorithms for solving algebraic Riccati-type equations. **Wen-Wei Lin** (National Tsing Hua University, Taiwan) IC/MT1384/020

Based on the doubling algorithm (Anderson 1978, Kimura 1988), we first propose a structure-preserving doubling algorithm (SDA) for computing the symmetric or symmetric positive semi-definite solution to the discrete-time algebraic Riccati equation (DARE), and the symmetric or symmetric positive definite to the nonlinear matrix equation (NME). The SDA algorithm is derived from a new point of view on doubling the associated symplectic pencil $(\mathcal{M}, \mathcal{L})$ while keeping the doubling pencil in a standard symplectic form at each step. We show that SDA converges quadratically if $(\mathcal{M}, \mathcal{L})$ has no unimodular eigenvalues, and it converges linearly with convergence rate 1/2 if all partial multiplicities of unimodular eigenvalues of $(\mathcal{M}, \mathcal{L})$ are even.

Secondly, we develop the SDA algorithm for the computation of the minimal nonnegative solutions to the nonsymmetric algebraic Riccati equation (NARE) and its dual equation, simultaneously. We establish a global quadratic convergence for SDA if the associated Hamiltonian-like M-matrix $\mathcal{K}$ is nonsingular, and a global linear convergence for SDA if the M-matrix $\mathcal{K}$ is irreducible and singular.

Numerical experiments show that the SDA algorithm is reliable, efficient, and outperforms QR-type, Newton-type methods on a set of benchmark problems.

IC/MP255/020: Computational methods for structured eigenvalue problems. #2

Organiser: Peter Benner (TU Chemnitz, Germany)
Co-organiser: Daniel Kressner (Umea University, Sweden)

(For abstract, see session #1 above.)

Numerical solution of eigenvalue problems with symplectic or palindromic structure. **Volker Mehrmann** (TU Berlin, Germany) IC/MT1139/020

We will discuss two different classes of eigenvalue problems (symplectic and palindromic) which have similar spectral properties. We will discuss their relationship and extend known results for symplectic and palindromic eigenvalue problems to matrix pencils and matrix polynomials. We present staircase algorithms for these classes to deflate singular parts and high index parts associated with the eigenvalue ∞.

We will also discuss numerical methods for the deflated prob-

lem that has only finite eigenvalues and semisimple infinite eigenvalues.

This is joint work with Ralph Byers, D. Steven Mackey, and Hongguo Xu

On a quadratic eigenvalue problem arising in the analysis of delay equations. **Heike Faßbender** (TU Braunschweig, Germany) IC/MT1393/020

The analysis of retarded linear m-delay time delay systems

$$\begin{array}{ll} \dot{x}(t) = \sum_{k=0}^{m} A_k x(t-h_k), & t > 0 \\ x(t) = \phi(t), & t \in [-h_m, 0] \end{array}$$

with $h_0 = 0 < h_1 < \ldots < h_m, x : [-h_m, \infty) \to \mathbb{R}^n, A_k \in \mathbb{R}^{n\times n}$, leads to a quadratic eigenvalue problem $Q(\lambda)u = 0$ where

$$Q(\lambda) = \lambda^2 E + \lambda F + G$$

with $E = A_m \otimes I, G = I \otimes A_m$, and $F = \sum_{k=0}^{m-1} I \otimes A_k e^{-i\phi_k} + A_k \otimes Ie^{i\phi_k}, \phi_k = \omega h_k$ where $\otimes$ denotes the Kronecker product. As there exists a permutation matrix P such that $P^T(A \otimes B)P = B \otimes A$ for all real $n \times n$ matrices A, B, the quadratic matrix polynomial Q satisfies

$$P^T rev(\overline{Q}(\lambda))P = Q(\lambda),$$

where $\overline{Q}(\lambda) = \lambda^2\overline{E} + \lambda\overline{F} + \overline{G}$ and $rev(Q(\lambda)) = \lambda^2 Q(\frac{1}{\lambda})$. Here we will discuss properties like eigenvalue pairing and structured linearization of such eigenproblems.

Work done in collaboration with Niloufer and Steve Mackey, Western Michigan University, Kalamazoo, MI 49008, USA.

Three numerical methods for the palindromic eigenvalue problem. **Christian Mehl** (TU Berlin, Germany) IC/MT2536/020

We discuss three numerical methods for the solution of the palindromic eigenvalue problem $Ax = \lambda A^T x$, where A is a complex matrix. Such eigenvalue problems occur, for example, in the vibration analysis of rail tracks. The first method is based on an idea that has been used by Laub for the solution of the Hamiltonian eigenvalue problem. The second method is a generalization of a non-symmetric Jacobi algorithm and the third method is a hybrid method that combines the best features of the first two methods, but also circumvents their failures.

This is joint work with D.S. Mackey, N. Mackey, and V. Mehrmann.

A numerical method for solving real Hamiltonian/skew-Hamiltonian eigenproblems. **Peter Benner** (TU Chemnitz, Germany) IC/MT4347/020

We discuss the computation of eigenvalues and deflating subspaces of real Hamiltonian/skew-Hamiltonian matrix pencils. Eigenproblems of this type arise in various application areas, in particular in linear-quadratic optimal control for descriptor systems and H_∞ optimization. In these applications, usually the stable deflating subspace, i.e., the subspace corresponding to the finite eigenvalues in the left half plane, is required.

The proposed algorithm is based on an embedding of the given matrix pencil in a Hamiltonian/skew-Hamiltonian pencil of double size for which a structured generalized Schur form can be computed. The method is efficient as it requires only about 2/3 of the computational effort the QZ algorithm would need to solve the original size generalized eigenproblem. We will also discuss the re-ordering of eigenvalues in detail as this is needed for obtaining the stable deflating subspaces required in the abovementioned applications.

IC/MP634/020: Preconditioners for sequences of linear systems.

Organiser: Philipp Birken (Universität Kassel, Germany)
Co-organiser: Jurjen Duintjer Tebbens (Academy of Sciences of the Czech Republic)

In many applications, not only one system of linear equations has to be solved, but a whole sequence of dozens, sometimes thousands of linear systems with different matrices and right hand sides obtained from the solution of previous systems.

Important examples are stiff differential equations or problems from optimization, where the appearing matrices are sparse and may be nonnormal. This minisymposium aims at discussing new techniques for solving these sequences of linear systems efficiently using preconditioned iterative methods. In particular, recently developed techniques that update preconditioners in contrast to freezing or recomputing them are considered.

The strategies to be addresses include approximate diagonal or triangular updates, recycled Krylov subspaces and Golub-Bartels types of updates.

An overview of efficient solution methods for sequences of linear systems. **Eric de Sturler** (Virginia Tech, USA) IC/MT3736/020

Many problems in science and engineering require the solution of a (long) sequence of linear systems. In order to solve such a sequence of systems efficiently, we want to reuse as much as possible previously calculated results. In addition to using the solutions of previous linear systems for an initial guess, we want to (1) *update* existing preconditioners to generate good preconditioners for subsequent problems at low cost, and (2) *recycle* search spaces from previous systems to improve the rate of convergence.

We will discuss several issues with respect to cost, effectiveness, and parallelism, and we will give an overview of current research in this area.

Updating incomplete factorizations for the solution of partial differential equations. **Jurjen Duintjer Tebbens** (Academy of Sciences of the Czech Republic), Daniele Bertaccini (Universita' di Roma "La Sapienza", Roma, Italy) IC/MT3473/020

The solution of algebraic linear systems of partial differential equations often requires the solution of sequences of large and sparse linear systems of the form

$$A_{\alpha_j} x = b, \qquad A_{\alpha_j} = A + \alpha_j E_j, \quad j = 0, \ldots, s, \quad \alpha_j \in \mathbf{C}, \qquad (1)$$

and E_j, $j = 0, \ldots, s$ are banded complex matrices.

These linear systems are often solved by iterative methods. However, without preconditioning these methods can converge very slowly and computing an incomplete factorization for each of the linear systems (1) can be costly and require memory space especially if s is large. On the other hand, reusing the same incomplete factorization strategy (e.g., computed for A) often leads to slow convergence. Clearly, there is a broad range of possibilities within these two extremes. We found a strategy for the update of an existing incomplete factorization preconditioner at a cost much lower than recomputing an incomplete factorization from scratch. Even if the resulting preconditioner can be expected to be less effective than a brand new one in terms of iteration count, the overall cost is, under suitable conditions, considerably reduced. The numerical solution of sequences of algebraic linear systems from the discretization of the real and complex Helmholtz equation and of

the diffusion equation illustrate the performance of the proposed approaches.

Sequences of linear systems as in (1) arise also in the numerical solution of the Helmholtz and of the Schrödinger equation; in large and sparse eigenvalues computation; in algorithms for nonlinear least squares and total least squares problems; in globalized quasi-Newton algorithms, etc.

Updating preconditioners for sequences of non-symmetric linear systems. **Philipp Birken** (Universität Kassel, Germany), Jurjen Duintjer Tebbens (Academy of Sciences of the Czech Republic), Andreas Meister (Universität Kassel, Germany), Miroslav Tůma (Czech Academy of Sciences, Czech Republic) IC/MT1578/020

The numerical solution of flows often leads to sequences of thousands of nonsymmetric linear systems with similar matrices and right hand sides. They are most currently solved with iterative methods preconditioned with ILU or other types of incomplete factorizations. The similarity of the matrices is exploited in praxis by recomputing the preconditioner not in every step, but periodically.

In this talk, a more sophisticated technique for nonsymmetric preconditioning is presented, where an incomplete LDU decomposition is updated in every step. The approach is algebraic and theoretically motivated. It generalizes diagonal updates previously introduced by Benzi and Bertaccini. Based on a reference LDU decomposition, the new preconditioner is computed via the difference between the current matrix and a reference matrix. This can be combined with a periodic recomputation of the reference preconditioner. It is demonstrated on several well-known testcases for the compressible Euler equations, that the new approach can reduce both CPU time and the total number of BiCGSTAB iterations.

Updating QR and LU factorizations in optimization. **Andreas Griewank** (Humboldt-Universität zu Berlin, Germany) IC/MT3498/020

In optimization algorithms approximating Jacobians and Hessians are frequently subject to low rank modifications due to changes in the active set or so called secant updates. In either case these corrections can be incorporated into QR or LU based factorizations at a cost that grows only linearly with the number of matrix entries. For square matrices dimension of n that means a cost of $O(n^2)$ rather than $O(n^3)$ for a complete refactorization. We review classical updating algorithms and observe that they may be unsatisfactory with regards to two criteria: data locality and asymptotic continuity. The first property is increasingly important for run time efficiency on modern computer architectures. The second properties means that the whole updating procedure reduces to the identity when the low rank meodifications tend to zero, which can be expected for secant updates.

IC/MP386/020: Preconditioning of symmetric indefinite systems in large-scale applications.

Organiser: Matthias Bollhöfer (TU Braunschweig, Germany)
Co-organiser: Olaf Schenk (Universität Basel, Switzerland)

One of the hardest challenges in the design of modern numerical solution methods is the design of robust and structure-preserving preconditioning techniques for highly symmetric indefinite linear systems, in particular those arising in PDE-constrained optimization or computational electronics based on Maxwell equations. Typically these problems require the computation of an approximate solution for systems which have up several million unknowns or larger due to their 3D spatial dimensions.
Continued advances in preconditioning techniques for symmetric indefinite systems and the ascendancy of modern software tools have in recent years motivated the use of these methods in large-scale applications.
In this minisymposium the first talk will address the computational challenges that arise in optimization with a focus on the preconditioning of symmetric indefinite linear systems, while the others will discuss theoretical and algorithmic advances for symmetric indefinite linear systems that arise from specific large-scale application problems such as PDE-constrained optimization and Maxwell problems. In particular the following aspects will be discussed:

- computational challenges that arise in large-scale optimization with focus on preconditioning of symmetric indefinite linear systems;
- Inertia-revealing preconditioning in large-scale nonconvex constrained optimization;
- augmentation techniques;
- implicit factorization preconditioners for KKT systems;
- KKT systems in optimal control of Magnetohydrodynamics;
- optimal control in large-scale constrained image construction;
- numerical challenges in industrial application problems arising from Maxwell equations;
- algebraic inverse-based preconditioning techniques for large-scale 2D/3D Helmholtz equations with high wave numbers.

Each topic is of interest in its own right. However, at the heart of each topic highly indefinite systems have to be solved numerically.

KKT systems arising in optimal control of magnetohydrodynamics. **Roland Griesse** (RICAM Linz, Austria) IC/MT1590/020

Magnetohydrodynamics (MHD) is a multi-physics phenomenon, dealing with the mutual interaction of electrically conducting fluids and magnetic fields. In particular, the magnetic fields interact with the electric currents in the fluid and exert a Lorentz force. This feature renders it so phenomenally attractive for exploitation especially in processes involving liquid metals, and in crystal growth.

The MHD forward or simulation problem has a saddle point structure, due to the constraints that the fluid velocity and current density be divergence free. The emphasis in this presentation will be on the large-scale linear systems arising in the simulation and optimal control of MHD, and their preconditioned iterative solution.

Preconditioners for distributed parameter-identification problems based on adaptive mesh refinement. **Eldad Haber** (Emory University, USA) IC/MT1781/020

In this talk we present an adaptive mesh discretization for distributed parameter identification problems. We then use this discretization in order to develop a highly efficient multigrid preconditioner for the systems which arise in the course of the constrained optimization algorithm.

Numerical challenges and industrial applications from frequency-domain simulations of Maxwell equations. **Stefan Reitzinger** (Computer Simulation Technology, Germany) IC/MT1288/020

In this talk we focus on the solution of Maxwell equations in frequency domain. Starting from a given 3D discretization of the full Maxwell equations, e.g. by the Finite Integration Technique (FIT), we end up with (depending on the boundary conditions and material properties) a sparse, large scale, indefinite, (non-)symmetric system matrix. This linear system has to be solved several times in a fast and robust way for different right hand sides. Because of the special properties of the Maxwell equations a "good" preconditioner has to be constructed very carefully. The construction of such a preconditioner based on algebraic multigrid principles is shown and additionally the numerical challenges are pointed out. Finally numerical studies from real life applications are presented.

Algebraic multilevel preconditioning for large-scale Helmholtz equations. **Matthias Bollhöfer** (TU Braunschweig, Germany) IC/MT1301/020

We discuss preconditioning methods for Helmholtz equation in two and three spatial dimensions with high wave number. In particular we present an algebraic multigrid algorithm that is based on three major ingredients, namely symmetric maximum weight matchings to increase the block diagonal dominance of the system, inverse-based pivoting to drive the coarsening process and finally filtering techniques to handle frequencies near zero eigenvalues. While the first two components can be considered as black-box approaches that can be widely used for preconditioning, the third component requires a more detailed adaption of the method to the underlying problem. I.e., in order to improve the coarsening process a pre-filtering method is applied prior to the inverse-pivoting approach.

IC/MP386/020: Preconditioning of symmetric indefinite systems in large-scale applications. #2

Organiser: Matthias Bollhöfer (TU Braunschweig, Germany)
Co-organiser: Olaf Schenk (Universität Basel, Switzerland)

(For abstract, see session #1 above.)

Numerical solution of saddle-point systems. **Jörg Liesen** (TU Berlin, Germany) IC/MT4741/020

Linear systems in saddle point form arise in numerous applications throughout computational science and engineering. No single best solution method for such systems exists. Rather, methods are typically constructed for the specific problem at hand. The ubiquitous nature of saddle point systems has led to an overwhelming variety of methods, with new methods appearing in the literature constantly. The goal of this talk is to provide an overview of existing solution methods, and some guidance in this vast area of scientific computing.

Inertia-revealing preconditioning for large-scale non-convex constrained optimization. **Olaf Schenk** (Universität Basel, Switzerland) IC/MT1226/020

We propose an inertia revealing preconditioning approach for the solution of nonconvex contrained optimization problems. If interior methods with second-derivative information are used for these optimization problems, a linearized Karush-Kuhn-Tucker system of the optimality conditions has to be solved. The main issue addressed is how to ensure that the Hessian is positive definite in the null-space of the constraints while neither adversely affecting the convergence of Newton's method or incurring a significant computational overhead. In the nonconvex case, it is of interest to find out the inertia of the current iteration system so that the matrix may be modified *a posteriori* to obtain convergence to a minimum.

However, in order to not destroy the rapid convergence rate of the interior method, the modification has only be performed in the cases where the inertia is not correct and factorization methods[3,4] are very often used in order to compute the inertia information. In this work, we propose a new inertia revealing preconditioned Krylov iteration to solve the linearized Karush-Kuhn-Tucker system of optimality conditions. Our preconditioning approaches for the symmetric indefinite Karush-Kuhn-Tucker systems are based on maximum weighted matchings and algebraic multi-level incomplete LBL^T factorizations[1,2]. Finally, we present numerical results on several large-scale three-dimensional examples of PDE-constrained optimizations in the full space of states, control and adjoints variables with equality and non-equality constraints and test them with artificial as well as clinical data from biomedical cancer hyperthermia treatment planning.

This is joint work with Andreas Wächter (IBM Research) and Martin Weiser (ZIB, Berlin, Germany).

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Augmentation preconditioners for saddle-point systems. **Chen Greif** (University of British Columbia, Canada) IC/MT1641/020

In this talk we provide an overview of augmentation preconditioners for saddle point systems of the form $[A\ B^T; B\ 0]$. Those preconditioners come in a few flavors. Defining W as a weight matrix, one basic form is block diagonal, with a weighted augmented matrix in the (1,1) block. The preconditioned matrix has the interesting property that the higher the nullity of the (1,1) block is, the faster a minimal residual Krylov solver (such as MINRES) converges. When the nullity of A is equal to the number of constraints, convergence (in the absence of roundoff errors) is expected to occur within two iterations. This preconditioning methodology fits certain situations in optimization quite well. For example, interior point solvers give rise to systems whose (1,1) block becomes increasingly ill-conditioned as the solution is approached.

Implicit factorizations for KKT systems. **Sue Dollar** (Rutherford Appleton Laboratory, UK) IC/MT1034/020

Each step of an interior point method for constrained optimization requires the solution of a system of equations which is symmetric, indefinite and takes the form

$$\begin{bmatrix} H & A^T \\ A & -C \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix} = \begin{bmatrix} c \\ d \end{bmatrix}.$$

Such a system is often called a KKT or saddle-point problem. As the problem size increases, the use of direct methods to solve this system may become prohibitively expensive and iterative methods become a viable alternative.

Dollar, Gould, Schilders and Wathen have recently proposed the use of implicitly defined constraint preconditioners when (approximately) solving KKT problems iteratively. These preconditioners only require the factorization of smaller systems and can be shown to give favourable Krylov subspace properties as well as allowing us to use a conjugate gradient-based iterative method. However, they often require a preprocessing step which carries out a symmetric permutation of the KKT problem. This permutation strongly relates to the problem of finding a nullspace basis of the linearized constraint space for the underlying optimization problem, but we'd also like to take additional characteristics of the Hessian into account when forming the permutation. We will discuss the desirable properties of such a permutation and how this might be achieved. Numerical experiments comparing several possible methods will be presented and it will shown that the more ill-conditioned the Hessian part of the KKT system is, the better the suggested preconditioners perform under suitable permutation choices.

This is joint work with Nick Gould, Wil Schilders and Andy Wathen.

IC/MP307/020: Numerical multilinear algebra: a new beginning.

Organiser: Pierre Comon (Université de Nice, France)
Co-organiser: Lieven De Lathauwer (CNRS-ETIS, France)
Co-organiser: Gene Golub (Stanford University, USA)
Co-organiser: Lek-Heng Lim (Stanford University, USA)

This minisymposium is on the development of numerical algorithms for multilinear algebra; a topic that is expected to have far-reaching applications in science and engineering, through both the creation of new scientific computing models and the analysis of data with nonlinear structures. The name *Numerical Multilinear Algebra* is not as yet in common usage. We broadly define this as the study and use of tensors/multilinear algebra, symmetric tensors/symmetric algebra, alternating tensors/exterior algebra, spinors/Clifford algebra in computational mathematics. A fundamental object of interest will be tensors. An order-k tensor may be either regarded as (1) a k-dimensional array of real/complex numbers on which algebraic operations generalizing analogous operations on matrices are defined, or (2) a linear combination of outer products of vectors. A matrix is then synonymous with a tensor of order 2. Special types of tensors such as symmetric and alternating tensors (arising from, say, cumulants and differential forms), Kronecker products of operators, are also of central importance. More specifically, this minisymposium will focus on numerical computations involving these multilinear objects, their surprising connections to questions regarding computational complexity and numerical stability, as well as the growing importance and increasing ubiquity of multilinearity in scientific and engineering applications.

The role of tensor rank in the complexity analysis of bilinear forms. **Dario Bini** (Universita' di Pisa, Italy) IC/MT3934/015

Three way-arrays (tensors) play an important role in the complexity analysis of sets S of bilinear form. In fact, the minimum number of (nonscalar) multiplications sufficient to compute S is given by the tensor rank of the three-way array $A = (a_{ijk})$ associated with S. Here, a tensor A has rank one if $A = (u_i \times v_j \times w_k)$ while it has rank at most $p > 1$ if there exist p rank-1 tensors T_i such that $A = T_1 + ... + T_p$.

Unlike matrices, there may exist sequences of tensors $\{A_p\}$ of given rank r which converge to a tensor of rank $r' > r$. This property has lead to the concept of border rank. While the tensor rank measures the complexity of computing sets of bilinear forms, the concept of border rank provides a measure of the complexity of approximating sets of bilinear forms.

In this talk, we provide an overview of known results concerning the complexity analysis of bilinear forms, discuss the role of multilinear algebra in this matter, present some extensions and list some open problems.

In particular, the concepts of tensor rank and border rank are revisited from a numerical point of view. Some criteria for giving lower bounds on the tensor rank and on the border rank of a given tensor are presented in terms of linear algebra tools, and their extensions to k-way arrays are discussed. Some examples are considered and a list of tensors whose (border) rank is still unknown is given.

Tensor computations for genomic signal processing. **Orly Alter** (University of Texas at Austin, USA) IC/MT3942/015

DNA microarrays make it possible to record the complete molecular biological signals that guide the progression of cellular processes on genomic scales. Biology and medicine today may be at a point similar to where physics was after the advent of the telescope [1]. The rapidly growing number of DNA microarray data sets holds the key to the discovery of previously unknown molecular biological principles, just as the astronomical tables compiled by Galileo and Brahe enabled accurate predictions of planetary motions and, later, the discovery of universal gravitation. Just as Kepler and Newton made these predictions and discoveries by using mathematical frameworks to describe trends in astronomical data, so future predictive power, discovery, and control in biology and medicine will come from the mathematical modeling of DNA microarray data, where the mathematical variables and operations represent biological reality: The variables, patterns uncovered in the data, might correlate with activities of cellular elements, such as regulators or transcription factors, that drive the measured signals. The operations, such as data classification and reconstruction in subspaces of selected patterns, might simulate experimental observation of the correlations and possibly also causal coordination of these activities. Such models were recently created from DNA microarray data by using the matrix computations of singular value decomposition (SVD) [2], generalized SVD (GSVD) [3] and pseudoinverse projection, and their ability to predict previously unknown biological as well as physical principles was demonstrated [4, 5]. I will now describe the first such data-driven models that were created from DNA microarray data by using tensor computations. First, I will describe the use of the matrix eigenvalue decomposition (EVD) and pseudoinverse projection and a tensor higher-order EVD in reconstructing the pathways that compose a cellular system from genome-scale nondirectional networks of correlations among the genes of the system [4]. Second, I will describe the use of a tensor higher-order SVD in integrating multiple datasets, corresponding to similar yet not identical biological studies of the same organism, and uncovering robust yet subtle differences among these datasets and corresponding studies. Third, I will describe the use of a tensor higher-order GSVD in comparing multiple datasets,

corresponding to similar biological studies of different organisms, and uncovering processes common or exclusive among these datasets and organisms.

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Finite-element differential forms. **Douglas Arnold** (University of Minnesota, USA), Richard Falk (Rutgers University, USA), Ragnar Winther (Universitetet i Oslo, Norway) IC/MT3961/029

A differential form is a field which assigns to each point of a domain in Euclidean space or, more generally, a manifold, an alternating multilinear form on its tangent space. The exterior derivative operation, which maps differential forms of one order to differential forms of the next higher order, unifies the basic first order differential operators of calculus, and is a building block for a great variety of differential equations. When discretizing such differential equations by finite element methods, stable discretization depends on the development of spaces of finite element differential forms. As revealed recently through the finite element exterior calculus, for each order of differential form, there are two natural families of finite element subspaces associate to a simplicial triangulation. In the case of forms of order zero, which is are simply functions, these two families reduce to one, which is simply the well-known family of Lagrange finite element subspaces of the first-order Sobolev space. For forms of degree 1 and of degree $n-1$ (where n is the space dimension), we obtain two natural families of finite element subspaces of $H(\mathrm{curl})$ and $H(\mathrm{div})$, unifying many of the known mixed finite element spaces developed over the last decades. This talk will concern the construction of such spaces, their properties and inter-relationships, and the construction of natural geometric bases for them, which generalize the Bernstein basis for Lagrange elements.

Multilinear algebra in machine learning and signal processing. **Lek-Heng Lim** (Stanford University, USA), Pierre Comon (Université de Nice, France) IC/MT4000/029

We will discuss how numerical multilinear algebra arises in both discriminative and generative models in machine learning: tensors in multilinear regression models (generalization of vector space models), symmetric tensors in independent component analysis, and nonnegative tensors in graphical models (ie. Bayesian networks). We will also introduce a multilinear spectral theory and show how the eigenvalues of symmetric tensors may be used to obtain basic results in Spectral Hypergraph Theory.

We will also discuss how the problem of blind source separation in signal processing may be solved either with the decomposition a data tensor into a sum of rank-one terms in the presence of sufficient diversity, or with the help of high-order statistics, namely cumulant tensors. In the latter case, the decomposition of the data cumulant, a symmetric tensor, into a linear combination of rank-one symmetric tensors can be used to extract factors when physical diversity does not allow direct and efficient storage of the data.

IC/MP307/020: Numerical multilinear algebra: a new beginning. #2

Organiser: Pierre Comon (Université de Nice, France)
Co-organiser: Lieven De Lathauwer (CNRS-ETIS, France)
Co-organiser: Gene Golub (Stanford University, USA)
Co-organiser: Lek-Heng Lim (Stanford University, USA)

(For abstract, see session #1 above.)

Fast multilinear approximation: a new generation of numerical algorithms. **Eugene Tyrtyshnikov** (Russian Academy of Sciences, Moscow) IC/MT3243/015

Large-scale problems arising in numerical mathematics and data analysis certainly need new approaches. Anyway we should look for some low-parametric "numerically viable" structure hidden in the data, and we are interested in some general tools that can help. A new generation of numerical algorithms can be based on fast construction of low-parametric multilinear (tensor) approximations both for the original problem and for all stages of an iterative solver. We demonstrate the new approximation tools and first implementations of this idea that may lead even to sublinear complexity.

Tensor-product decomposition in computational physics. **Boris Khoromskij** (Max-Planck-Institut Leipzig, Germany) IC/MT3321/015

Modern methods of tensor-product decomposition allow an efficient data-sparse approximation to integral and more general nonlocal operators in higher dimensions (cf. [1] – [7]). Examples of such nonlocal mappings are classical volume potentials, solution operators of elliptic/parabolic BVPs, spectral projection operators associated with the matrix *sign* function for solving the Hartree-Fock equation in electronic structure calculations, collision integrals from the deterministic Boltzmann equation as well as the convolution integrals from the Ornstein-Zernike equation in molecular dynamics.

We discuss the approximation theory and numerical methods of structured low tensor-rank approximation to function-related tensors and operators based on the Tucker and canonical models. The asymptotic complexity of such approximations can be estimated by $O(\log^{pd} n + dn\log^q n)$ with $p \le 1$, where $N = n^d$ is the discrete problem size (hence, avoiding the "curse of dimensionality"). In particular, we consider applications to the classical Newton, Yukawa and Helmholtz potentials, to the multi-variate functions $\frac{1}{|x-y|^y}$ and $e^{-\alpha|x-y|^y}$ with $x, y \in \mathbb{R}^d$, as well as to the elliptic operator inverse. Numerical results will be addressed.

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Separated representations and nonlinear approximations for fast algorithms in high dimensions. **Gregory Beylkin** (University of Colorado at Boulder, USA) IC/MT3914/015

As is well known, representing functions in an appropriate basis facilitates the solution of linear differential and integral equations. However, in nonlinear problems the role of bases is limited, since linear combinations of solutions are not solutions. Moreover, in high dimensions, representations via bases may have far too many components and, thus, their utility is questionable. As an alternative to bases we may use optimal or optimized representations of functions. In particular, we have been using separated representations as a tool for solving linear and nonlinear equations in high dimensions, with the optimization applied to reduce the number of terms in the approximation. We present examples of separated representations, nonlinear approximations, and the associated numerical algorithms.

Fast Newton-type methods for non-negative tensor approximation. **Inderjit Dhillon** (University of Texas at Austin, USA) IC/MT5040/015

Nonnegative Tensor Approximation is an effective decomposition technique that is useful in a wide variety of applications ranging from document analysis and image processing to bioinformatics. There are existing algorithms for nonnegative tensor approximation (NNTA), for example, Lee & Seung's multiplicative updates, alternating least squares, and certain gradient-descent based procedures. However, all these procedures suffer from slow convergence or numerical instabilities. In this talk, I will present improved algorithms for the NNTA problem, which overcome many computational deficiencies of existing methods. In particular, our methods use non-diagonal gradient scaling for faster convergence. These methods provide numerical results that are superior to both Lee & Seung's method as well to the alternating least squares (ALS) heuristic, which is known to work well in some situations but has no theoretical guarantees. I will present experimental results on both synthetic and real-world datasets to demonstrate the effectiveness of the new methods, in terms of better approximations as well as computational efficiency.

IC/MP271/020: Solution methods for sequences of linear systems and applications.

Organiser: Eric de Sturler (Virginia Tech, USA)

The simulation and optimization of systems arising in science and engineering often result in the solution of a sequence of linear systems where the matrix and possibly the right hand side(s) are changing. In some cases, such as crack propagation, thousands of systems must be solved. In many cases, the matrix changes slowly from one system to the next, and the changes often have special structure. For these applications, we can reduce the overall solution time drastically by exploiting the slowly changing nature of the matrices. For this reason, there is currently significant interest in developing linear solvers and preconditioners for sequences of linear systems. Several methods have been succesfully applied in applications ranging from tomography, the optimization of large structures, materials science, and stochastic finite elements for uncertainty quantification. This minisymposium aims to bring together both developers of solvers and researchers applying these solvers.

Solving sequences of linear systems: recent advances. **Eric de Sturler** (Virginia Tech, USA) IC/MT2722/020

We will start with an overview of methods that accelerate the solution of a sequence of linear systems by reusing information that is available from previous systems, and we discuss typical applications. After that we briefly discuss Krylov recycling for a sequence of symmetric linear systems and an application in topology optimization for optimal structures and advanced materials design. This is joint work with Glaucio Paulino and Shun Wang (UIUC).

Adaptive preconditioners for nonlinear systems of equations. **Daniel Loghin** (University of Birmingham, UK) IC/MT2767/020

The use of preconditioned Krylov methods is in many applications mandatory for computing efficiently the solution of large sparse nonlinear systems of equations. However, the available preconditioners are often sub-optimal due to the changing nature of the linearized operator. In this work we introduce and analyze an adaptive preconditioning technique based on the Krylov subspace information generated at previous steps in the nonlinear iteration. In particular, we use an adaptive technique suggested for restarted GMRES to enhance existing preconditioners with information available from previous Arnoldi factorizations computed in the course of the nonlinear iteration. Numerical tests drawn from the areas of optimization and nonlinear PDEs are used to illustrate the increased efficiency of our approach.

Physics-based preconditioners for solving PDEs on highly heterogeneous media. **Burak Aksoylu** (Louisiana State University, USA), Hector Klie (University of Texas at Austin, USA) IC/MT3335/020

Eigenvalues of smallest magnitude become a major bottleneck for iterative solvers especially when the underlying physical properties have severe contrasts. These contrasts are commonly found in many applications such as composite materials, geological rock properties and thermal and electrical conductivity. The main objective of this work is to construct a method as algebraic as possible that could efficiently exploit the connectivity of highly heterogeneous media in the solution of diffusion operators. We propose an algebraic way of separating binary-like systems according to a given threshold into high- and low-conductivity regimes of coefficient size $O(m)$ and $O(1)$, respectively where $m \gg 1$. The condition number of the linear system depends both on the mesh size Δx and the coefficient size m. For our purposes, we address only the m dependence since the condition number of the linear system is mainly governed by the high-conductivity subblock. Thus, the proposed strategy is inspired by capturing the relevant physics governing the problem. Based on the algebraic construction, a two-stage preconditioning strategy is developed as follows: (1) a first stage that comprises approximation to the components of the solution associated to small eigenvalues and, (2) a second stage that deals with the remaining solution components with a deflation strategy (if ever needed). The deflation strategies are based on computing near invariant subspaces corresponding to smallest and deflating them by the use of recycled Krylov subspace projections. Due to its algebraic nature, the proposed approach can support a wide range of realistic geometries (e.g., layered and channelized media). Numer-

ical examples show that the proposed class of physics-based preconditioners are more effective and robust compared to a class of Krylov-based deflation methods on highly heterogeneous media.

Subspace recycling for image-reconstruction applications. **Misha Kilmer** (Tufts University, USA), Eric de Sturler (Virginia Tech, USA) IC/MT2750/020

The need to solve a sequence of large-scale linear systems involving matrices whose characteristics vary slowly from one subsequent system to the next arises frequently in image reconstruction problems. In tomography applications (electrical impedance or diffuse optical tomography), for example, one often needs a nonlinear forward model in the form of a discretized partial differential equation (PDE) to describe the relationship between the desired quantity (e.g. a 3D image of the diffusion of light in tissue) and the measured data. To find the desired image requires the solution of a nonlinear optimization problem for the unknown voxel values in the image, which in turn requires the solution of multiple linear systems (the discretized PDEs) – one or more such systems in each iteration of the optimization algorithm. Even in applications where a linear forward model is used, sequences of systems can arise from time processing of data, or from sewing slices of information together to produce 3D images.

In this talk, we analyze matrix characteristics and techniques for reducing the computational complexity of the sequence of systems arising in tomography applications. In particular, we derive strategies for recycling Krylov subspace information that exploit properties of the application and the nonlinear optimization algorithm to significantly reduce the total number of iterations over all linear systems. Although we focus on a particular application, our approach is applicable generally to problems where sequences of linear systems must be solved. Examples illustrate the promise of our approach in reducing the overall computational complexity of nonlinear image reconstruction problems.

IC/MP271/020: Solution methods for sequences of linear systems and applications. #2

Organiser: Eric de Sturler (Virginia Tech, USA)

(For abstract, see session #1 above.)

Krylov-subspace recycling in stochastic finite-element computations. **Elisabeth Ullmann** (TU Bergakademie Freiberg, Germany), Oliver Ernst (TU Bergakademie Freiberg, Germany) IC/MT3324/020

A popular variant of the stochastic finite element method requires the solution of a large number of parametrized linear systems of equations. The associated coefficient matrices are linear combinations of a small number of finite element stiffness matrices resulting from coefficient functions which are eigenfunctions of a covariance operator. Since these parametrized matrices are closely related in this way, it is to be expected that Krylov subspace recycling techniques are able to efficiently reuse subspaces generated in the course of solving one equation for the approximation of other solutions.

In this talk we report our experience with Krylov subspace recycling techniques in combination with GCROT as well as a MINRES-like solver for families of Hermitian systems in a variety of stochastic finite element computations.

Analysis of Krylov-subspace recycling for sequences of linear systems. **Michael Parks** (Sandia National Laboratories, USA), Eric de Sturler (Virginia Tech, USA) IC/MT2763/020

We review a class of Krylov subspace methods for sequences of linear systems, which reduce the cost of solving the next system in the sequence by "recycling" information from previous systems. These methods have been successfully applied to sequences of linear systems arising from several different application areas. We analyze a particular method that recycles nearly invariant subspaces, and establish residual bounds that suggest a convergence rate similar to one obtained by removing select eigenvector components from the initial residual. Both symmetric and nonsymmetric problems are considered, and numerical experiments illustrating the effects of subspace recycling are presented.

Domain-decomposition preconditioned recycling GMRES algorithms for stochastic partial differential equations. **Xiao-Chuan Cai** (University of Colorado at Boulder, USA) IC/MT2746/020

In this talk, we discuss some parallel multilevel Schwarz-type domain decomposition preconditioned recycling Krylov subspace method for the numerical solution of some partial differential equations with stochastic uncertainties in the operator. Using a Karhunen-Loeve expansion and double orthogonal polynomials, we transform the stochastic problem into a large number of related, but uncoupled deterministic equations. To solve the systems efficiently, "recycling of computation" is the key. We report some interesting results obtained from a PETSc based parallel implementation of a recycling Krylov subspace method with a domain decomposition preconditioning. This is a joint work with C. Jin and C. Li.

Flexible GMRES with deflated restarting with application to a solution of the Helmholtz equation. **Xavier Pinel** (CERFACS, France), Luc Giraud (ENSEEIHT, France), Serge Gratton (CERFACS, France), Xavier Vasseur (CERFACS, France) IC/MT5029/020

In this talk we will describe a flexible Krylov subspace method that enables the preconditioner to change from one iteration to the next. It is referred to Flexible GMRES-DR due to its close ressemblance with the GMRES-DR method by R. Morgan in the way it recycles some spectral information at each restart. Numerical experiments for the solution of the Helmholtz equations using the multigrid scheme by Riyanti *et al.* as preconditioner will be reported.

This is joint work with L. Giraud (ENSEEIHT-IRIT), S. Gratton (CERFACS) and X. Vasseur (CERFACS).

IC/MP4145/020: Structured matrix algorithms: new methods.

Organiser: Olga Holtz (TU Berlin, Germany & UC Berkeley, USA)
Co-organiser: Plamen Koev (Massachusetts Institute of Technology, USA)
Co-organiser: James Demmel (UC Berkeley, USA)

Numerous applications in sciences and engineering, as well as in computational, applied and pure mathematics give rise to problems involving matrices with Toeplitz, Hankel, Vandermonde, Cauchy structures, along with many other patterns of structure. Standard mathematical software tools are mostly based on structure-ignoring methods, and therefore their use is often not appropriate for obtaining a satisfactory solution. Indeed, ignoring the structure can potentially increase the storage from $O(n)$ to $O(n^2)$ and increase the running time from $O(n)$ to $O(n^3)$, depending on the structure. Secondly, many structured matrices are extremely ill-conditioned, which means that all available standard methods may fail to produce even one correct digit in the computed solution. The only way to overcome these difficulties is to exploit the special structure of such matrices, and to design more efficient algorithms.

Fast linear algebra is stable. **James Demmel** (UC Berkeley, USA), Olga Holtz (TU Berlin, Germany & UC Berkeley, USA), Ioana Dumitriu (University of Washington, USA) IC/MT4023/020

We show that a large class of fast recursive matrix multiplication algorithms are stable in a normwise sense, and that if multiplication of $n \times n$ matrices can be done by any algorithm in $O(n^w)$ operations, then it can be done stably in $O(n^{w+e})$ operations for any $e > 0$. We extend this to show that many standard linear algebra operations, including LU and QR decomposition, linear equation solving, matrix inversion and determinant computation can also be done stably in $O(n^{w+e})$ operations.

Novel structured and unstructured preconditioners. **Victor Pan** (Lehman College, CUNY, USA) IC/MT1811/020

We propose a novel approach to preconditioning for solving linear systems of equations and some other fundamental matrix computations. Our preconditioners are readily available for quite a general class of ill conditioned matrices, with no preliminary information about the SVD, and can be chosen to preserve and exploit the structure of the input matrix. We describe various techniques for computing with our preconditioners, link them to the aggregation methods, and analyze them theoretically and experimentally.

Fast algorithms for polynomial Vandermonde matrices related to quasi-separable matrices. **Thomas Bella** (University of Connecticut, USA), Vadim Olshevsky (University of Connecticut, USA), Yuli Eidelman (Tel Aviv University, Israel), Israel Gohberg (Tel Aviv University, Israel) IC/MT3982/020

While general matrix algorithms are known to require $O(n^3)$ operations, the special structure of Vandermonde and Vandermonde-related matrices allows computational savings resulting in algorithms of only $O(n^2)$ operations for certain special classes. Specific classes that have already been considered are classical Vandermonde matrices, Chebyshev-Vandermonde matrices, three-term Vandermonde matrices, and Szegö-Vandermonde matrices. In each the known algorithms for inversion and for solving a linear system are of the lower $O(n^2)$ complexity. In this paper we consider the most general special class of quasiseparable-Hessenberg-Vandermone matrices that generalize all the above classes. We derive generalizations of the well-know Bjorck-Pereyra and Traub algorithms. The results of numerical experiments will be presented.

A quadratically-convergent method for solving certain Riccati equations based on structured matrix technology. **Dario Bini** (Universita' di Pisa, Italy) IC/MT3282/020

Structural and computational properties of Cauchy-like matrices are used for the design and analysis of algorithms for solving certain matrix Riccati equations encountered in transport theory. We provide an algorithm with complexity $O(n^2)$ ops per step having quadratic convergence, where n is the size of the matrix which solves the equation. The possibility of reducing the computational cost to $O(n)$ ops, up to polylog factors, is discussed.

IC/MP712/020: Structured matrix algorithms: complexity and stability.

Organiser: Olga Holtz (TU Berlin, Germany & UC Berkeley, USA)
Co-organiser: Plamen Koev (Massachusetts Institute of Technology, USA)
Co-organiser: James Demmel (UC Berkeley, USA)

Numerous applications in sciences and engineering, as well as in computational, applied and pure mathematics give rise to problems involving matrices with Toeplitz, Hankel, Vandermonde, Cauchy structures, along with many other patterns of structure. Standard mathematical software tools are mostly based on structure-ignoring methods, and therefore their use is often not appropriate for obtaining a satisfactory solution. Indeed, ignoring the structure can potentially increase the storage from $O(n)$ to $O(n^2)$ and increase the running time from $O(n)$ to $O(n^3)$, depending on the structure. Secondly, many structured matrices are extremely ill-conditioned, which means that all available standard methods may fail to produce even one correct digit in the computed solution. The only way to overcome these difficulties is to exploit the special structure of such matrices, and to design more efficient algorithms.

Over the last decade, numerically stable and fast methods have been developed for several classes of structured matrices (e.g., Cauchy, Vandermonde and generalized Vandermonde, matrices with low displacement rank). These new methods are being incorporated into software and libraries such as MATLAB and LAPACK. The proposed mini-symposium will bring together pure and applied mathematicians and software developers working on theoretical and computational problems involving structured matrices. This will create a unique opportunity to discuss advances and challenges in the area of structured matrix problems.

Structured matrices and reproducing-kernel spaces. **Harry Dym** (Weizmann Institute of Science, Israel) IC/MT2747/020

The purpose of this talk is to highlight the natural connections that exist between structured matrices and certain classes of reproducing kernel spaces. The link is made by interpreting the matrix as the Gram matrix of the space, which will be a finite dimensional Hilbert space if the given matrix is positive definite and a finite dimensional Krein space if the matrix is Hermitian and invertible. This connection has important implications in assorted problems of bitangential interpolation and factorization, as will be illustrated by examples. The talk will be expository.

Linear and multilinear structures in matrix approximation. **Eugene Tyrtyshnikov** (Russian Academy of Sciences, Moscow) IC/MT2628/020

Two important general types of structure in matrices include linear (like Toeplitz, etc.) and multilinear (low-rank matrices) structure. Previously both types have been studied separately. However, one can benefit a lot of a combination of both types of structure. Eventually it may lead to considerable reduction in number of representation parameters. Also, it opens up a new line for construction of preconditioners; i.e., *best circulant preconditioners* and far-reaching generalizations of the same approach.

Accurate algorithms for structured eigenvalue problems. **Froilán Dopico** (Universidad Carlos III de Madrid, Spain) IC/MT1981/020

In the last years an intense research effort has been done to identify special classes of matrices where very accurate spectral computations are possible and to develop efficient algorithms to perform these high accurate computations. At present many classes of symmetric matrices, definite or indefinite, deserving a high relative computation of their eigenvalues are known, but only two classes of nonsymmetric matrices have been identified. The main ideas behind these algorithms are: to choose for each class of matrices a set of parameters that determines its eigenvalues accurately, i.e., small relative perturbations of the parameters produce small relative changes in the eigenvalues, and to restrict some of the operations performed by the algorithms to accurate operations on the parameters. The purposes of this talk are: to present a unified overview on these algorithms and to present the most recent developments in this area.

Bidiagonal decomposition of totally positive Bernstein–Vandermonde matrices. **José-Javier Martínez** (Universidad de Alcala, Spain), Ana Marco (Universidad de Alcala, Spain) IC/MT3448/020

The class of Bernstein–Vandermonde matrices (a generalization of Vandermonde matrices arising when the monomial basis is replaced by the Bernstein basis) is considered. A convenient ordering of their rows makes these matrices strictly totally positive.

By using results related to total positivity and Neville elimination, an algorithm for computing the bidiagonal decomposition of a Bernstein-Vandermonde matrix is constructed. The use of explicit expressions for the determinants involved in the process serves to make the algorithm both fast and accurate.

One of the applications of our algorithm is the design of fast and accurate algorithms for solving Lagrange interpolation problems when using the Bernstein basis, an approach useful for the field of computer aided geometric design since it avoids the stability problems involved with basis transformations between the Bersntein and the monomial bases.

A different application consists of the use of the bidiagonal decomposition as an intermediate step of the computation of the eigenvalues and the singular value decomposition of a totally positive Bernstein-Vandermonde matrix.

IC/MP712/020: Structured matrix algorithms: complexity and stability. #2

Organiser: Olga Holtz (TU Berlin, Germany & UC Berkeley, USA)
Co-organiser: Plamen Koev (Massachusetts Institute of Technology, USA)
Co-organiser: James Demmel (UC Berkeley, USA)

(For abstract, see session #1 above.)

Quasi-separable matrices and polynomials. **Vadim Olshevsky** (University of Connecticut, USA), Thomas Bella (University of Connecticut, USA), Israel Gohberg (Tel Aviv University, Israel), Yuli Eidelman (Tel Aviv University, Israel) IC/MT3964/020

Quasi-separable matrices are garnereing a lot of attention recently. Several results and algorithms for polynomials associated with quasiseparable matrices will be presented

Computing structured pseudospectra. **Daniel Kressner** (Umea University, Sweden) IC/MT3072/020

In the presence of high non-normality, the eigenvalues of a matrix or linear operator are not always helpful in understanding features of the underlying application. For example, the linear approximation of a dynamical system may have all eigenvalues far-off in the left half plane, even though the original system is unstable. In contrast, pseudospectra and related concepts (e.g., the pseudospectral radius) remain robust under uncertainties in the matrix and sometimes represent a more appropriate means to gain insights, e.g., on stability questions. In this talk, we consider structured pseudospectra, which arise if the uncertainties are known to preserve certain properties of the matrix. Computational aspects for the following classes of structured matrices are discussed: real matrices, skew-symmetric matrices, and Hermitian matrices. In all three cases, it turns out that computing one point of the structured pseudospectrum requires the solution of an eigenvalue minimization problem. Using appropriate reformulations and block Lanczos methods, it is shown how these minimization problems can be solved within a complexity that grows only quadratically with the matrix order and, hence, the computational cost is not much higher than for unstructured pseudospectra. Based on this work, a graphical user interface for computing structured pseudospectra, similar to Tom Wright's Eigtool, is being developed. This is joint work with Michael Karow.

Bayesian analysis of stability of structured matrix algorithms. **Daniela Calvetti** (Case Western Reserve University, USA) IC/MT3192/020

In this talk we analyse the stability of a few classes of structured matrix algorithms from the Bayesian perspective. In particular, we are interested in tracking how uncertainties in the initial data propagate to the computed solutions. Tools from Bayesian inference will be used to express uncertanty in terms of random variables. By using sampling methods we will present pointwise predictive envelopes for the output of the algorithms.

How does Matlab exploit matrix structure?. **Cleve Moler** (The MathWorks, Inc., USA) IC/MT1439/020

MATLAB does not have any specific "structured matrix" data type. This talk will examine how and where MATLAB does take advantage of various kinds of matrix structure – real versus complex, symmetry, positive definiteness, sparseness, bandedness, Toeplitz, Hankel, etc.

IC/MP672/020: Mathematical topics in matrix iterations.

Organiser: Marko Huhtanen (Teknillinen Korkeakoulu, Finland)
Co-organiser: Olavi Nevanlinna (Teknillinen Korkeakoulu, Finland)

This minisymposium deals with various mathematical problems related to iterative methods. Its partial purpose is to emphasize that advances in iterative methods do not result only from considering immediate applications. Even seemingly pure mathematical studies can lead to practical algorithms and approaches. In this type of research, tools and methods from many fields, such as complex and real analysis, operator and approximation theory, algebraic geometry, are needed.

GMRES and complex approximation theory. **Anne Greenbaum** (University of Washington, USA) IC/MT3579/020

Questions about the convergence of the GMRES algorithm for solving a linear system whose coefficient matrix is a Jordan block are related in an interesting way to certain problems in complex approximation theory. In [*The polynomial numerical hulls of Jordan blocks and related matrices*, Lin. Alg. Appl. 374 (2003), pp. 231-246] Faber, et. al. used an old result of Schur and Szegö about polynomial approximation to prove a new result about the polynomial numerical hull of degree $n-1$ for an n by n Jordan block and hence about the convergence of the GMRES algorithm applied to such a matrix. In [*GMRES convergence and the polynomial numerical hull for a Jordan block*, submitted to Lin. Alg. Appl.], Liesen and Tichý proved still more results about the convergence of the GMRES algorithm applied to a Jordan block and these, in turn, imply interesting new results about the behavior of polynomials in the complex plane. In this paper we show the connection between these seemingly different subjects and use the known results in each area to establish new results in the other.

Matrix nearness problems and iterative methods. **Marko Huhtanen** (Teknillinen Korkeakoulu, Finland) IC/MT2320/020

In this talk we consider measuring the deviation of $A \in \mathbb{C}^{n\times n}$ from unitarity in a more refined way by looking at

$$\min_{W\in\mathcal{U},F\in\mathcal{F}_k} ||A-F-W||,$$

for $k = 0,1,2,\ldots,n-1$. Here $\mathcal{U}$ denotes the set of unitary matrices and $\mathcal{F}_k$ matrices of rank k at most. Analogously to the way the singular values of A express how A is stratified away from zero, these numbers measure the deviation from unitarity in a more refined way.

Matrix iterative methods and potential theory. **Arno Kuijlaars** (Katholieke Universiteit Leuven, Belgium) IC/MT2099/020

Conjugate Gradients and the Lanczos method are basic iterative algorithms in numerical linear algebra. They belong to a class of Krylov subspace methods whose convergence properties can be described by a polynomial approximation problem. For large size matrices the approximation problem is analyzed with techniques from logarithmic potential theory. The theoretical results give good predictions for the convergence rates of the numerical methods.

Convergence of two-sided minimum residual iterations. **Olavi Nevanlinna** (Teknillinen Korkeakoulu, Finland) IC/MT2386/020

A two-sided minimum residual method was introduced[1] for problems of the form

$$(I+S)x = b$$

where fast operating with both S and S^{-1} are simultaneously available. In this talk we discuss the asymptotic convergence properties of such processes, suitably modifying the existing theory[2,3].

[1] Huhtanen, Marko and Nevanlinna, Olavi; A minimum residual algorithm for solving linear systems. BIT 46: (2006) pp.533–548.

[2] Nevanlinna, Olavi; *Convergence of Iterations for Linear Equations*. Birkhauser, 1993.

[3] Nevanlinna, Olavi; *Meromorphic Functions and Linear Algebra*. Fields Institute Monographs, AMS, 2003.

IC/MP347/020: Model reduction: structured and higher-order systems.

Organiser: Volker Mehrmann (TU Berlin, Germany)
Co-organiser: Roland Freund (UC Davis, USA)
Co-organiser: Zhaojun Bai (UC Davis, USA)

Model order reduction is currently one of the fundamental research areas in simulation and control of large-scale systems. Despite recent progress in the development of Krylov subspace methods, SVD-based methods, and POD methods, in most practical applications there is a discrepancy between fast and efficient methods to compute the reduced order model, preservation of physical properties of the system, like conservation laws, stability, passivity, or variational properties of the system.

There is a lot of research activity in this direction and it is the aim of this minisymposium to bring some of the key players in academia and industry together, to exchange the latest developments and to coordinate research activities. We focus on the preservation of structure, like that of symmetric or higher-order systems.

Numerical and semi-analytical structure-preserving model reduction for MEMS. **David Bindel** (Courant Institute, NYU, USA) IC/MT998/020

Micro-electro-mechanical systems (MEMS) devices usually involve interactions between different types of physics, which leads to meaningful structures in the models of these devices. These device models also frequently have subsystems which correspond to physical components about which the designer may have some intuition or prior knowledge. In this talk, we describe how the HiQLab simulator for resonant MEMS supports the construction of reduced models that preserve these structures. In particular, we describe how designers can describe, at a high level, subsystems that should be preserved in a Krylov subspace based reduced model. We also describe how HiQLab easily allows users to define global shape functions to augment or replace automatically-generated bases for the different substructures. We give examples of structure-preserving reduced models of high-frequency resonant MEMS which we have constructed as part of our study of damping in these devices.

Structure-preserving model reduction without using explicit projection. **Roland Freund** (UC Davis, USA) IC/MT1002/020

In recent years, there has been a lot of progress in Krylov subspace-based structure-preserving model reduction of large-scale linear dynamical systems. However, all existing methods first generate a basis matrix of the underlying Krylov subspace and then employ explicit projection using some suitable partitioning of the basis matrix to obtain a structure-preserving reduced-order model. There are two major problems with the use of such explicit projections. First, it requires the storage of the basis matrix, which becomes prohibitive in the case of truly large-scale linear dynamical systems. Second, the approximation properties of the resulting structure-preserving reduced-order models are far from optimal, and they show that the available degrees of freedom are not fully used. In this talk, we discuss Krylov subspace-based recduction techniques that do not require explicit projection and thus overcome the two major problems of projection methods.

Robust algorithms for parametric model order reduction. **Lihong Feng** (TU Chemnitz, PR China), Peter Benner (TU Chemnitz, Germany) IC/MT1140/020

In many engineering applications, physical models contain some parameters. Parametric systems can be used to describe for example geometry and/or material variations in the physical system. The goal of parametric model order reduction is to preserve the parameters in the reduced-order model. Using the parametric reduced-order model, one can do quick simulations with different values of the parameters with acceptable error.

This paper is based on the work by Daniel (2004), where a parametric model reduction method is proposed that resembles the AWE method for moment matching. Here, we will propose a robust numerical algorithm for realizing this method. We develop an algorithm which computes the moments of the parametric system implicitly rather than explicitly. The method can be interpreted as an Arnoldi-type method using a modified Gram–Schmidt implementation. In this way, good numerical stability properties can be expected as an orthonormal basis of the projection subspace (which is needed for computing accurate projectors for model order reduction) can be obtained. The proposed algorithm can deal with both single-input and multi-input linear parametric systems without limitation on the number of parameters in the system. Simulation results show that our algorithms are very promising for various engineering problems.

Solvability and numerical methods for quadratic model updating problems. **Wen-Wei Lin** (National Tsing Hua University, Taiwan) IC/MT1181/020

Model updating problem (MUP) concerns the modification of an existing but inaccurate analytical model with measured data. For models characterized by quadratic pencils, the measured data usually involve incomplete knowledge of natural frequencies, mode shaps, or other specral information. In conducting the updating we have two viewpoints in solving MUP.

(I) We incorporate the measured modal data in the analytical model producing an adjusted model on the mass, damping and stiffnes, that closely match the experimental modal data. The new methods are direct methods, which require $O(nk^2)$ flops, and employ sparse matrix technique when the analytical model is sparse. Here n is the size of coefficient matrices defining the analytical model and k is the number of measured eigenpairs.

(II) We match the desired measured data without tampering with the other part of unmeasured or unknown eigenstructure inherent in the original model. Such an updating, if possible, is said to be no spill-over, which is a challenging task in applications. WE provide a complete theory on when such an updating with no spill-over is possible.

IC/MP348/020: Model reduction in circuit simulation.

Organiser: Volker Mehrmann (TU Berlin, Germany)
Co-organiser: Zhaojun Bai (UC Davis, USA)
Co-organiser: Roland Freund (UC Davis, USA)

Model order reduction is currently one of the fundamental research areas in simulation and control of large-scale systems. Despite recent progress in the development of Krylov subspace methods, SVD-based methods, and POD methods, in most practical applications there is a discrepancy between fast and efficient methods to compute the reduced order model, preservation of physical properties of the system, like conservation laws, stability, passivity, or variational properties of the system.

There is a lot of research activity in this direction and it is the aim of this minisymposium to bring some of the key players in academia and industry together, to exchange the latest developments and to coordinate research activities. We focus on new and more efficient model reduction techniques in circuit simulation.

Model compiler, model order reduction and circuit simulation. **Richard Shi** (University of Washington, USA) IC/MT4180/020

This talk presents some latest progresses in model order reduction in circuit simulation. The specific emphasis is how a model compiler can be explored to analyze the underlying model structures and to direct efficient model order reduction.

Model order reduction for linear and nonlinear circuit simulation in nanoscale IC electronics. **Jan ter Maten** (NXP Semiconductors, The Netherlands), Arie Verhoeven (Technische Universiteit Eindhoven, The Netherlands), Thomas Voss (TU Delft, The Netherlands), Tamara Bechtold (NXP Semiconductors, The Netherlands), Wil Schilders (NXP Semiconductors, The Netherlands) IC/MT4188/020

Simulation for nanoelectronics requires that circuit equations are coupled to electromagnetics, semiconductor equations, and involves heat transfer. Model Order Reduction (MOR) is a means to speed up simulation of large systems. Existing MOR techniques have to be generalized to be applicable to the resulting system of (Partial) Differential-Algebraic Equations (DAEs, PDAES). Also nonlinearity and parameterization have to be taken into account. They are the key points to make MOR applicable in industrial simulation and occur in three related MOR topics: behavioural modeling (for use in system design), nonlinear and parameterized MOR (for use in the main simulations), and approximation methods using response surface techniques for robust design (for use in optimization). With respect to nonlinear systems, Proper Orthogonal Decomposition (POD) methods as well as extensions of the balanced truncation methods have recently been developed. We studied a generalization to DAEs based on least squares techniques. To reduce costs in evaluations Missing Point Estimation (MPE) was studied. The idea is to build a nonlinear reduced order model by projecting a part of the original equations onto the subspace spanned by the chosen set of basis functions. The technique has been successfully applied to partial differential equation (PDE) models and to reduce successfully a DAE model of an inverter chain model. The same DAE model was also considered to study Trajectory Piece-Wise Linear (TPWL), combined with "PoorMan's TBR" to reduce the locally linearized systems,

created along a typical time-domain trajectory of the original system, and compiling a weighted overall linearized system. The time points for updating the local Krylov basis are determined dynamically, based on error control. Combining the bases gives a POD-like approximation that allows to use linearized problems. We will also address several experiences with inclusion of parameters.

Approaches for model reduction of PDE-described systems. **Luca Daniel** (Massachusetts Institute of Technology, USA), Jacob White (Massachusetts Institute of Technology, USA) IC/MT4189/020

In applications as diverse as nano-photonics, bioMEMS, and aircraft design, system designers need approaches for automatically extracting dynamically-accurate and computationally-efficient models from partial-differential-equation (PDE) descriptions. The problem of extracting reduced models from arbitrary systems of PDE's is already extremely difficult, but system designers often need even more. Extracted models are most useful to designers when these models are parametric, and can therefore include the performance impact of manufacturing variations.

The standard approach to model reduction of PDE systems is to first discretize in space, and then convert the problem to a very large system of ordinary differential equations. If the resulting dynamical system is linear, then existing reduction techniques can be applied, albeit with modifications to address the infeasibility of directly factoring the resulting huge system matrices. For parameterized and nonlinear PDE's, the landscape of methods is far less well resolved, perhaps because the general problem is almost certainly intractable. There are some techniques that work well for very specific problems, but the limitations and the accuracy of these techniques have yet to be properly characterized. In this talk, the authors will give examples of several recently developed techniques, with the hope of inspiring a more concerted effort at better understanding the topic's theoretical underpinnings.

Parameterized interconnect macromodeling via a 2D Arnoldi process. **Yangfeng Su** (Fudan University, PR China), Zhaojun Bai (UC Davis, USA) IC/MT4192/020

A Krylov subspace projection method is proposed for the model-order reduction of large scale parameterized interconnect networks. The reduced system is constructed via a novel two-dimensional Arnoldi process such that it matches a prescribed number of the multiparameter moments. We call it the PIMTAP algorithm, which stands for Parameterized Interconnect Macromodeling via a Two-dimensional Arnoldi Process. The PIMTAP algorithm inherits the advantages of the existing multiparameter moment-matching methods, such as multivariable Taylor series method and the CORE method, and avoids the shortfalls of these methods. It is computationally stable and robust and preserves the structure and therefore the passivity of the original parameterized interconnect network.

IC/MP348/020: Model reduction in circuit simulation. #2

Organiser: Volker Mehrmann (TU Berlin, Germany)
Co-organiser: Zhaojun Bai (UC Davis, USA)
Co-organiser: Roland Freund (UC Davis, USA)

(For abstract, see session #1 above.)

Model order reduction techniques from an application point-of-view in high-frequency simulations. **Stefan Reitzinger** (Computer Simulation Technology, Germany) IC/MT1290/020

In this talk we focus on model-order reduction techniques for two types of applications:
(a) Given a 3D discretization of the full Maxwell equations, e.g. by the Finite Integration Technique (FIT), the aim is to construct a much smaller model such that the S-parameters are well approximated up to a userdefined accuracy. A fast, robust and reliable solution exists via a band Lanczos method, where loss-free and weakly lossy structures can be calculated. However extensions to general lossy (e.g. lossy metal) and parameter dependent problems are required.
(b) Second, given a set of discrete S-parameters from, e.g. a Time Domain calculation. We would like to approximate the given S-parameters by a linear time invariant (LTI) system which is as small as possible, stable and passive in the whole frequency range. The difficulties for this application are (in general) the non-passive S-parameters and as a consequence the enforcement of passivity during the approximation process. In addition the set of S-parameters can be very large. Finally we would like to construct a SPICE list out of the LTI system which is as small as possible. The mentioned difficulties and possible solutions to them are discussed.

Work done in collaboration with M. Elger and P. Thoma, CST GmbH Darmstadt.

Passivity-preserving model reduction of differential-algebraic equations in circuit simulation . **Tatjana Stykel** (TU Berlin, Germany), Timo Reis (TU Berlin, Germany) IC/MT2001/020

We consider model order reduction of linear differential-algebraic equations arising in circuit simulation. We present an extension of the positive real and bounded real balanced truncation model reduction methods for such equations that are based on balancing the solutions of projected generalized Lur'e and Riccati matrix equations. Important properties of these methods are that stability and passivity are preserved in the reduced-order model and that there exist approximation error bounds. Numerical solution of the corresponding matrix equations using the special structure of circuit equations is also discussed.

Model order reduction techniques for linear systems with large numbers of terminals. **Peter Feldmann** (IBM T.J. Watson Research Center, USA) IC/MT4156/020

This contribution addresses the well-known difficulty of applying model order reduction (MOR) to linear circuits with a large number of input-output terminals. Traditional MOR techniques substitute the original large but sparse matrices used in the mathematical modeling of linear circuits by models that approximate the behavior of the circuit at its terminals, and use significantly smaller matrices.

Unfortunately these *small* MOR matrices become dense as the number of terminals increases, thus canceling the benefits of size reduction. The paper introduces a model reduction technique suitable for circuits with numerous terminals. The technique exploits the correlation that almost always exists be-

tween circuit responses at different terminals. The correlation is rendered explicit through an SVD-based algorithm and the result is a substantial sparsification of the MOR matrices. The proposed sparsification technique is applicable to a large class of problems encountered in the analysis and design of interconnect in VLSI circuits. Relevant examples are used to analyze and validate the method.

Parameterized and nonlinear MOR in the simulation of RF circuits . **Wil Schilders** (NXP Semiconductors, The Netherlands) IC/MT4179/020

IC design automation tools are indispensable for RF designers in the transition to the nano-scale era. These tools are needed to develop nano-scale designs of unprecedented complexity and performance and, in addition, enable the achievement of single-pass design success to avoid costly re-spins and the loss of market opportunities. Next generation designs will be challenged by an increased number of trouble spots, many of which negligible at lower frequencies but representing a significant limitation for future designs. These trouble spots will have to be accounted for during the design phase in order to avoid costly mishaps that can originate potential failures and additional design and silicon iterations, and must be addressed in future design automation tools.

The key to the avoidance of these trouble spots is the recognition that devices can no longer be treated in isolation. Complete RF blocks must be considered as one entity. Today, it is not possible to perform such analyses of complete RF blocks. The CHAMELEON RF project will deliver the methodologies and prototype tools to make this possible. The results will lead to design automation tools, in particular design verification tools, that can be used for comprehensive and highly accurate modeling of electromagnetic effects and other trouble spots in complete nano-scale RF blocks, thereby enabling designers to minimize turnaround time without compromising design quality and first-time-right requirements.

In the presentation, an overview will be given of the methods that are being developed within the CHAMELEON-RF project (see: http://www.chameleon-rf.org), and that will enable a fully coupled solution of RF blocks. The emphasis will be on model order reduction techniques for interconnected and parameterized systems, and some recent results on nonlinear MOR will also be presented.

IC/MP347/020: Model reduction: structured and higher-order systems. #2

Organiser: Volker Mehrmann (TU Berlin, Germany)
Co-organiser: Roland Freund (UC Davis, USA)
Co-organiser: Zhaojun Bai (UC Davis, USA)

(For abstract, see session #1 above.)

Approximation and recovery of damped-wave operators. **Mark Embree** (Rice University, USA) IC/MT3098/020

Damped wave equations are canonical examples of second-order dynamical systems whose discretizations lead to structured first-order linear systems driven by non-symmetric matrices. In practice one may wish to determine material properties of a physical system based on measurements of vibration. In this talk, we shall describe a approximate technique for recovering spatially-dependent viscous damping from spectral data. As a natural consequence of this construction, one can estimate the number of eigenvalues that should be accurately captured by a reduced order model for this physical system. Numerical results will be compared to high-precision measurements taken from a monochord in our string laboratory. (This talk describes collaborative work with Steven J. Cox of Rice University.)

Advances in model reduction of structured dynamical systems. **Zhaojun Bai** (UC Davis, USA) IC/MT4088/020

In this talk, under a unified theory, we review our recent work on model reduction methods for structured dynamical systems. These include RLC/RCS interconnect circuits, even and palindromic systems in large scale optimal control and bilinear systems arising from bilinearization of nonlinear dynamical systems.

This is a joint work with Rencang Li, Volker Mehrmann, Daniel Skoogh, Yangfeng Su, Hongguo Xu and Xuan Zeng.

Nonlinear model order reduction methods for oscillatory systems and their applications. **Jaijeet Roychowdhury** (University of Minnesota, USA) IC/MT4089/020

The lack of fast yet accurate oscillator and PLL simulation methods has constituted a serious bottleneck in mixed-signal, RF and digital design flows. We will describe methods that, given differential equations for any oscillator (ie, equivalent to, eg, a SPICE-level circuit), will extract a simple nonlinear phase macromodel. We will show how such nonlinear phase macromodels are capable of capturing a variety of important effects, including jitter and phase noise, injection locking, PLL lock and capture phenomena, cycle slipping, etc., while being faster by several orders of magnitude than SPICE-level simulation. Time permitting, we will also show how this nonlinear phase macromodel, when applied to large systems of networked biochemical and and nanoelectronic oscillators, correctly predicts spontaneous pattern formation and edge detection.

Entropy-based empirical relations between original and reduced state variables. **Patricia Astrid** (Shell Global Solutions International B.V, The Netherlands) IC/MT4168/020

In projection-based model reduction methods, the reduced basis which approximates the original dynamics is derived from the main dynamical features inferred from the collected state variable evolutions, controllability, or observability Gramians. However, the relations between original and reduced state variables are not explicitly available since all original state variables are entangled in the reduced basis. This paper presents an empirical method developed from the Shannon Entropy concept which identifies the individual relations between the original and reduced state variables. The empirical relations are applied in the closed loop control design of a spatio-temporal model reduced by the POD method. The incorporation of the empirical relations in the closed loop design results in a more effective closed loop performance.

IC/MP353/020: Numerical linear algebra in image processing.

Organiser: James Nagy (Emory University, USA)
Co-organiser: Misha Kilmer (Tufts University, USA)

Digital images are used to analyze objects in a variety of applications, such as star clusters in astronomy, molecules in biology, and tumors in medicine. Often the process used to obtain the image cannot be easily repeated, and the collected data must be used to reconstruct, restore or enhance the image. These processes often require the solution and/or analysis of challenging computational linear algebra problems. For example, special techniques must be used for very large linear systems that arise in three dimensional imaging applications, as well as for applications that require solution of constrained optimization problems. Often matrix approximations and fast algorithms for structured matrices must be employed. Due to advances in technology, the development of new imaging devices, and the desire to obtain images with ever higher resolution, research in these areas is extremely active. The speakers in this minisymposium will report on recent developments in numerical linear algebra models and algorithms that have been developed for tackling challenging problems in image processing.

Super-resolution methods for multi-lenslet iris-imaging system. **Victor Pauca** (Wake Forest University, USA), Todd Torgersen (Wake Forest University, USA) IC/MT3236/020

Multi-lenslet imaging systems offer a number of significant advantages over standard single-lens camera systems, including thin form-factor and wide angle of view. By using appropriate lenslet spacing relative to the detector pixel pitch, the resulting ensemble of images implicitly contains subject information at higher spatial frequencies than those present in a single image. Additionally, a multi-lenslet approach enables the use of observational diversity, including phase, polarization, neutral density, and wavelength diversities. For example, post-processing multiple observations taken with differing neutral density filters can yield an image having an extended dynamic range. As a part of the DTO-funded PERIODIC project, our research group has developed several multi-lens camera prototypes for the investigation of such diversities. In this talk, we present recent results obtained by our research group on superresolution of iris imagery using novel multi-lens imaging systems and iterative methods for (sequential and joint) registration and reconstruction. More specifically, we compute high-resolution reconstructed images from ensembles of low-resolution images containing sub-pixel level displacement diversity. Quality of the reconstructed images is measured in terms of biometric identification for iris recognition, by computing the Hamming distance between the Daugman iris code of a conventional reference iris image, and the iris code of a corresponding reconstructed image. We present numerical results concerning the reconstruction of actual iris data obtained with our camera prototypes.

Multilevel regularization for image deblurring problems. **Marco Donatelli** (Università degli Studi dell'Insubria Como, Italy) IC/MT1659/020

We consider the de-blurring problem of noisy and blurred signals/images in the case of space invariant point spread functions. The use of appropriate boundary conditions leads to linear systems with structured coefficient matrices related to space invariant operators like Toeplitz, circulants, trigonometric matrix algebras etc. We combine an algebraic multigrid (which is designed ad hoc for structured matrices) with the low-pass projectors typical of the classical geometrical multigrid employed in a PDEs context. Thus, using an appropriate smoother, we obtain an iterative regularizing method based on: projection in a subspace where it is easier to distinguish between the signal and the noise and then application of an iterative regularizing method in the projected subspace. Therefore any iterative regularizing method can be used as smoother in our multigrid algorithm. The projector is chosen in order to maintain the same algebraic structure at each recursion level and having a low-pass filter property, which is very useful in order to reduce the noise effects. In this way, we obtain a better restored image with a flatter restoration error curve and also in less time than the auxiliary method used as smoother. As direct consequence the choice of the exact iteration where to stop is less critical than in other regularizing iterative methods.

Work done in collaboration with S. Serra-Capizzano.

Multilevel approaches for the total least-squares method in deblurring problems. **Malena Español** (Tufts University, USA), Misha Kilmer (Tufts University, USA), Dianne Oleary (University of Maryland, USA) IC/MT2569/020

In some image deblurring applications, complete knowledge of the blurring operator is unavailable. Thus, the inverse problem of recovering the deblurred image in the presence of noise is complicated by the need to model the uncertainty in the blurring operator, adding to the computational complexity of the inversion. Regularized total least squares approaches have been presented in the literature which require the minimization of a functional with respect to the unknown perturbation in the blurring operator, the residual, and the desired image. However, much of the work to date has required the perturbation operator to have special structure (e.g. sparsity structure or Toeplitz type structure) in order to make the minimization problem more computationally tractable. We present a multilevel approach to the regularized total least squares problem which allows us to remove this operator restriction and still has the advantage of computational speed. Examples illustrate the potential effectiveness of our approach.

Cascadic multilevel methods for ill-posed problems. **Lothar Reichel** (Kent State University, USA) IC/MT3616/020

Multilevel methods are popular for the solution of well-posed problems, such as certain boundary value problems for partial differential equations and Fredholm integral equations of the second kind. However, little is known about the behavior of multilevel methods when applied to the solution of linear ill-posed problems, such as Fredholm integral equations of the first kind, with a right-hand side that is contaminated by error. We discuss properties of cascadic multilevel methods with a conjugate gradient-type method as basic iterative scheme. In particular, we consider applications to image deblurring and denoising using edge-preserving prolongation operators based on partial differential equations defined by Perona-Malik and total variation-type models. The talk presents joint work with Serena Morigi, Fiorella Sgallari, and Andriy Shyshkov.

IC/MP353/020: Numerical linear algebra in image processing. #2

Organiser: James Nagy (Emory University, USA)
Co-organiser: Misha Kilmer (Tufts University, USA)

(For abstract, see session #1 above.)

Antireflective deblurring. **Martin Hanke** (Universität Mainz, Germany) IC/MT1207/020

We consider the numerical solution of selfadjoint deblurring problems on bounded intervals. For these problems it has recently been shown that appropriate modelling of the solution near the boundary of the interval may significantly improve the numerical reconstructions. Among the alternatives the so-called antireflective boundary condition appears to be the best known choice. Here we develop an appropriate, i.e., stable and efficient implementation of this model in two steps, namely by (i) transforming the problem to homogeneous boundary values, and (ii) using the fast sine transform to solve the transformed problem. This approach allows to incorporate regularization in a very straightforward way. Numerical reconstructions are superior to those obtained with the reblurring method of Donatelli and Serra-Capizzano.

Wave-front estimation for adaptive optics systems on ground-based telescopes. **Johnathan Bardsley** (University of Montana, USA) IC/MT1818/020

The earth's atmosphere is not a perfect media through which to view objects in outer-space; turbulence in the atmospheric temperature distribution results in refractive index variations that interfere with the propagation of light. As a result, wavefronts are non-planar when they reach the ground. The deviation from planarity of a wavefront is known as phase error, and it is phase error that causes the refractive blurring of images. Adaptive optics systems seek to remove phase error from incoming wavefronts. In ground-based astronomy, an estimate of the phase error in a wavefront is typically obtained from wavefront gradient measurements collected by a Shack-Hartmann sensor. The estimate is then used to create a counter wavefront, e.g. using a deformable mirror, which (approximately) removes the phase error from the incoming wavefronts. The problem of reconstructing the phase error from Shack-Hartmann gradient measurements requires the solution of a large linear system. This system is defined by the configuration of the Shack-Hartmann sensor. We derive its form and then present several effective computational methods Ű both old and new Ű for its solution.

A modified GCV method for Lanczos hybrid regularization. **Julianne Chung** (Emory University, USA), James Nagy (Emory University, USA) IC/MT1338/020

Lanczos hybrid regularization methods have been proposed as effective approaches to solve large-scale ill-posed inverse problems. Regularization parameters must be chosen at each iteration. In this talk, we describe a modified generalized cross validation scheme for this purpose. Some theoretical results are given, and numerical experiments show that the modified GCV method is effective at choosing regularization parameters.

A parameter-choice method that exploits residual information. **Per Christian Hansen** (Danmarks Tekniske Universitet, Denmark), Misha Kilmer (Tufts University, USA) IC/MT3711/020

Most algorithms for choosing the regularization parameter in a discrete ill-posed problem are based on the norm of the residual vector. We present a new approach, where we seek to use all the information available in the residual vector. We present important relations between the residual components and the amount of information that is available in the noisy data, and we show how to use statistical tools and fast Fourier transforms to extract this information efficiently. This approach leads to a computationally inexpensive parameter-choice rule based on the normalized cumulativeperiodogram, which is particularly suited for large-scale problems.

IC/MP131/020: Developments in algebraic multigrid methods for real-world applications.

Organiser: Luke Olson (Univ. of Illinois at Urbana-Champaign, USA)
Co-organiser: Scott MacLachlan (TU Delft, The Netherlands)

As the demand for more complex computational simulations continues to grow, so do the challenges imposed on the underlying numerical algorithms. This minisymposium highlights recent progress in the numerical solution of the large, sparse linear systems that arise in simulation of real-world applications. In particular, recent advances in algebraic multigrid (AMG) methods are considered in four areas of interest to the practitioner: theoretical analysis, parallel robustness, feasibility for advanced discretizations, and practical industrial application.

Algebraic multigrid has been established as an effective solution technique for a wide variety of problems. Improving its viability as an optimal or near-optimal black-box solver (yielding $\mathcal{O}(n)$ growth in complexity for $n \times n$ systems of equations) in real-world simulations requires a closer look at several challenges posed by traditional approaches. Simulations of complex, three-dimensional, real-world applications provide a motivational base for continued research. The challenges of accurately modelling the underlying physics coupled with the practical demands of simulation provide unique challenges to AMG. Simulation in high-performance environments, for example, is a common roadblock and both the AMG setup and solve phases are impacted in a parallel setting. Further, while standard finite-element discretizations are amenable to multigrid iteration, less conventional paradigms, such as high-order discontinuous spectral methods, offer significant advantages in terms of accuracy per degree of freedom. Better understanding of these challenges, both computationally and theoretically, provide a solid base for the practitioner.

The principle goal of this minisymposium is to outline these challenges and the associated progress towards more robust, efficient, and well-understood algebraic multigrid solution methods for real-world applications.

Practical aspects of theoretical bounds on algebraic multigrid. **Scott MacLachlan** (TU Delft, The Netherlands), Luke Olson (Univ. of Illinois at Urbana-Champaign, USA) IC/MT3760/020

Algebraic multigrid (AMG) techniques offer optimal performance as solvers or as preconditioners for many large-scale linear systems that arise in modern applications. Many of these applications, however, exhibit strongly heterogeneous characteristics that preclude analysis using classical techniques such as Fourier analysis. In this talk, we introduce AMG and discuss the challenges of deriving good theoretical bounds on its performance. In particular, we consider challenges in making practical choices in the algorithmic components based on theoretical analysis.

Theoretical bounds on AMG performance come with many different conditions and assumptions, reflecting AMG's many variants and options. For the practitioner, however, it is desirable to have a simple sharp bound that accurately reflects the choices made in constructing the AMG grid and operator hierarchies. The questions of sharpness and computability of existing bounds on AMG convergence are thus considered. The role in which recent advances in adaptive AMG and compatible relaxation play in these bounds is also discussed. Despite these and other advances, the challenge of deriving useful bounds for complex applications subject to limitations of computer architectures remains distant; our viewpoint suggests possibilities for research to achieve this goal.

Algebraic multigrid for high-order discretizations. **Luke Olson** (Univ. of Illinois at Urbana-Champaign, USA) IC/MT3359/020

The use of high-order spectral and finite elements in the numerical approximation to partial differential equations continues to grow in popularity. In many situations, the accuracy per degree of freedom when using high-order elements surpasses the low-order approach. The total computational cost, however, requires a deeper investigation of the complexity in the full simulation tool chain. In this talk, we focus on a common and nontrivial component of the process: solution of the associated algebraic system of equations. In particular, we highlight an algebraic-based multigrid (AMG) preconditioner for nodal elements on rectangular meshes as well as unstructured simplex meshes in both two and three dimensions [1,2].

For simplex meshes we consider high-order nodal spectral elements based on the electrostatic and Fekete distributions and tensoral GLL nodes in the case of rectangular grids. A low-order finite element preconditioner over a local tessellation of the element is constructed. We detail the use of AMG in this context for elliptic problems and investigate the performance. Notably, by utilizing the low-order AMG preconditioner, the solution process maintains optimal complexity for moderately high-order elements ($p = 12$ in 2D and $p = 10$ in 3D). Furthermore, with a modified AMG preconditioner, we are able to achieve similar performance for nonconforming discretizations such as the local discontinuous Galerkin method.

[1] L. N. Olson, *Algebraic Multigrid Preconditioning for High-Order Discontinuous Spectral Elements*, SIAM J. Sci. Comput., 2006, submitted.

[2] Heys, J. J., Manteuffel, T. A., McCormick, S. F., Olson, L. N., *Algebraic Multigrid for Higher-Order Finite Elements*, J. Comput. Phys. 204 (2005), no. 2, 520-532.

Markov chains and web ranking: a multilevel adaptive aggregation method. **Hans De Sterck** (University of Waterloo, Canada) IC/MT1993/020

Google's PageRank method for ranking web pages models how a *random surfer* follows links between web pages in a random fashion. The stationary probability vector of the resulting Markov chain provides a ranking of all the pages in the network. Calculating this stationary probability vector is a very large problem: Google now indexes more than 25 billion internet web pages. We present a multilevel adaptive aggregation method for the linear algebra problem of calculating the stationary probability vector of a Markov chain. The method described is a variant of adaptive algebraic multigrid methods for sparse linear systems, and is also related to existing aggregation methods for Markov chains. We apply our multilevel method to a set of stochastic matrices that provide models for web page ranking. These numerical tests serve to illustrate for which types of stochastic matrices our multilevel adaptive method may provide significant speedup compared to standard iterative methods. The tests also provide some insight into why the PageRank model is a successful model for determining a ranking of web pages.

On the use of algebraic multigrid methods in surgery simulations of complex geometries like the human head. **Jens Schmidt** (NEC Europe, Germany) IC/MT3492/020

We are dealing with the simulation of maxillo-facial surgeries, especially with distraction osteogenesis. During this treatment the surgeon cuts free the patient's upper jaw (maxilla), which is subsequently relocated into a new position in the course of several weeks, using a distraction device.The presented simulation toolchain is set up to predict the displacements of the facial tissues during and after the pulling process and is based on individual CT images of the patient's head before treatment. Its purpose is to support the surgeon in optimizing the treatment plan and avoiding additional post operative plastic surgeries.The input data for the simulation toolchain is generated by adding the suggested cuts, the geometry of the distraction device and the suggested forces to the CT data of the patient's head. From these data we generate a Finite Element mesh of the head and perform a Finite Element analysis of the distraction process.

In order to achieve sufficient accuracy we have to resolve most of the geometrical features of the human head, which leads to a large number of unknowns, typically several million. In addition the computational costs are significantly increased by the size of the displacements and the visco-elastic behaviour of the materials, which can only be properly approximated by non-linear modeling. The image processing, the meshing and the analysis of the model are run via a grid service on an HPC resource. Focusing on the efficiency of the simulation, the linear solvers used to solve the arising systems of equations play the most crucial role. In our case standard iterative solvers like Krylov methods or ILU methods fail, as we will show in our presentation. Therefore we will focus on the use of Multigrid solvers.

But the complex geometry of the human head in combination with large jumps of the material parameters (Young's modulus jumps about 5 orders of magnitude between bone and soft tissues) prevents standard multigrid approaches from converging at a sufficient rate. In theory convergence can be dramatically improved by computing the *near null space* of the systems, consisting of quasi-rigid body modes, and treating it separately. We will show the limitations of this approach for highly complex geometries, like the human head.In our presentation we will demonstrate the performance of three AMG-based solvers we have found to work on our problems: BoomerAMG from LLNL's hypre package [1], ML from Sandia's Trilinos package [2] (based on smoothed aggregation) and the PARDISO package [3] from the University of Basel, Switzerland (based on algebraic multilevel incomplete LDL^T factorizations). We will show the results of our intensive parameter studies and discuss the extensibility of our performance results for elasto-mechanical Finite Element simulations in general.

[1] http://www.llnl.gov/CASC/hypre/software.html

[2] http://software.sandia.gov/trilinos/

[3] http://www.computational.unibas.ch/cs/scicomp/software/pardiso/

IC/MP268/020: Matrix functions: methods and applications.

Organiser: Valeria Simoncini (Dipartimento di Matematica, Universita' di Bologna, Italy)
Co-organiser: Andreas Frommer (Bergische Universität Wuppertal, Germany)

The approximation of matrix functions has received significant attention during the past few years, resulting in great advances in the numerical treatment as well as in the use of matrix functions in applied sciences. The aim of this minisymposium is to gather leading researchers in the subject to present recent developments in the study of numerical methods for the approximation and use of matrix functions.

Effects of non-normality on the behavior of matrix functions. **Anne Greenbaum** (University of Washington, USA) IC/MT3578/020

The behavior (in 2-norm) of a function of a normal matrix A, such as $\exp(A)$ or A^k, is determined by the eigenvalues of A. This is not so for nonnormal matrices, and we discuss other properties of such matrices that one might look at in order to estimate $\|f(A)\|$ for various functions f. Possibilities include the field of values, pseudospectra, polynomial numerical hulls, matrices that are similar to A via a well-conditioned similarity transformation, and more diagonally dominant matrices that are unitarily similar to A. We discuss the theory and application of several of these ideas.

Restarted Krylov-subspace approximation of matrix functions. **Stefan Güttel** (TU Bergakademie Freiberg, Germany), Oliver Ernst (TU Bergakademie Freiberg, Germany), Michael Eiermann (TU Bergakademie Freiberg, Germany) IC/MT3067/020

Approximating the product of a function $f(A)$ of a matrix A with a vector b is a key task in many scientific computing applications. When the matrix A arises from the discretization of a differential or integral operator, methods based on the direct factorization become too expensive and Krylov subspace projection methods become attractive. One shortcoming of this methodology, however, is its large storage requirements when a large number of iteration steps are required for a sufficient approximation.

Recently, we proposed a technique for restarting a Krylov subspace calculation resulting in fixed storage requirements which can be specified *a priori*. In this talk we present an enhancement of this method which reduces the amount of computation in the subspace calculation based on an updated Schur factorization. We compare the resulting algorithm with the previous one for several numerical examples.

Gaussian quadrature rules for second-order finite-difference schemes. **Vladimir Druskin** (Schlumberger Ltd., USA), Leonid Knizhnerman (Central Geophysical Expedition, Russian Federation), Liliana Borcea (Rice University, USA), Fernando Guevara Vasquez (Stanford University, USA) IC/MT2037/020

To evaluate $f(A)b$, Krylov subspace methods approximate A by small structured matrices T, in particular, by a tri-diagonal matrix, that matches some moments of the spectral measure of A. One can consider A as a one-dimensional second order differential operator and T as the matrix of the three-point (second order) finite-difference (FD) operator with a specially chosen grid [Druskin, Knizhnerman, SINUM, **37**, 2, 2000, 403-426], hence the name FD Gaussian rules (FDGR). The grids generated by the FDGR are also called optimal for shorthand. The most remarkable property of the optimal grids is exponential convergence of the transfer (also known as spectral or Weyl) function of the FD operator at the boundary of the domain, but globally the scheme converges with first or second order. With the help of tensor-product grids and domain decomposition this property can be transformed to exponential superconvergence of multidimensional second order FD approximations at targeted points or manifolds. Another important property of the optimal grids is their weak dependence on distribution of coefficients for certain classes of PDEs. We discuss applications of the FDGR to the solution of forward and inverse PDE problems arising in oil exploration and medical imaging.

An acceleration technique for the numerical solution of certain matrix equations. **Beatrice Meini** (Università di Pisa, Italy) IC/MT1264/020

Consider the matrix function:

$$\mathcal{R}(X) = XCX - XD - AX + B, \qquad (1)$$

where A, B, C, D are real matrices of sizes $m \times m, m \times n, n \times m, n \times n$, respectively, such that

$$M = \begin{bmatrix} D & -C \\ -B & A \end{bmatrix}$$

is an irreducible singular M-matrix, and X is real of size $m \times n$. The matrix function $\mathcal{R}(X)$ has applications in transport theory and Markov models. The interest is the computation of the minimal nonnegative solution X_+ of the equation $\mathcal{R}(X) = 0$. The latter equation is a nonsymmetric algebraic Riccati equation (NARE).

We introduce a new approach to treat the singularity of M based on a shift technique. The shift consists in performing a rank-one correction of the matrix M which moves one zero eigenvalue to a suitable nonzero real number. We construct a new matrix function $\tilde{\mathcal{R}}(X)$ which defines a NARE associated with the shifted M, which has the same solution X_+ of the original one, while the coefficients of the new Riccati equation form a nonsingular matrix if 0 is a simple eigenvalue of M.

The performances of various algorithms applied to the original and to the shifted Riccati equations are analyzed. In particular, it is proved that the convergence of the SDA (Structure Preserving Doubling) algorithm is accelerated when it is applied to the shifted Riccati equation.

IC/MP268/020: Matrix functions: methods and applications. #2

Organiser: Valeria Simoncini (Dipartimento di Matematica, Universita' di Bologna, Italy)
Co-organiser: Andreas Frommer (Bergische Universität Wuppertal, Germany)

(For abstract, see session #1 above.)

Computing functions of matrices via quadrature and conformal maps. **Lloyd Trefethen** (University of Oxford, UK) IC/MT2669/020

One of the most powerful and flexible tools for computing $f(A)$, where A is a matrix or operator, is a Cauchy integral. By using suitable variable transformations related to the IMT and DE methods of Mori and others, these algorithms can be made very fast indeed. A crucial part of their analysis is interpreting the transformations as conformal maps.

We will describe recent progress in this area, partly joint work with Nick Higham.

Recent advances in the implementation of exponential integrators. **Marlis Hochbruck** (Universität Düsseldorf, Germany) IC/MT3774/020

The efficiency of exponential time integration schemes strongly depends on the algorithms used for evaluating or approximating the product of a matrix function an a vector.

In this talk we will discuss various options for computing $f(A)b$ which may be incorporated into existing algorithms:

1. We consider the approximation of the product of a matrix function with a set of vectors, $f(A)b_i$, $i = 1,\ldots,s$, using Krylov subspace methods. We assume that A is a constant matrix and that the vectors b_i correspond to the evaluation of a smooth function at certain quadrature nodes. This problem arises in the implementation of exponential integrators, in which case f is related to the exponential function. We propose a projection technique and analyse its properties. Our analysis gives rise to a new practical stopping criterion for the iteration. Moreover, we present numerical examples which show a significant gain in computational time compared to a naive implementation, where a new Krylov basis is computed for each vector b_i.
2. For solving linear systems of equations with subspace iterations, restarts are a well established tool. Recently, Eiermann and Ernst showed how restarts can be incorporated into the evaluation of $f(A)b$. We will give an alternative derivation which might help to understand the convergence behavior of these approximations.

This is joint work with Jörg Niehoff.

Function of structured matrices in geometric integration of ODEs. **Luciano Lopez** (Universita' di Bari, Italy) IC/MT1472/020

In this talk we present methods for evaluating the exponential function at structured matrices like skew-symmetric and/or Hamiltomian ones. These results are essentially motived by the study of geometric integrators for solving ODEs evolving on matrix groups like the orthogonal or symplectic group, where the numerical solution is required to lie on the same matrix group of the theoretical solution. By exploiting the particular form of these structured matrices we may derive effective methods which preserve the exponential function on the associated matrix group. The possibility to use Krylov subspaces methods in the context of geometric integrator is also investigated.

Numerical methods for the QCD overlap operator: hybrid Monte-Carlo with overlap fermions. **Thomas Lippert** (Forschungszentrum Jülich, Germany), Nigel Cundy (Universität Regensburg, Germany), Andreas Frommer (Bergische Universität Wuppertal, Germany), Stefan Krieg (Forschungszentrum Jülich, Germany) IC/MT3754/020

The use of chiral (e.g., overlap) fermions offers an intriguing possibility for the simulation of QCD at small masses. The computational costs of calculating the sign of the Wilson matrix within the overlap operator did so far not allow to simulate on realistic, four dimensional lattices, using dynamical overlap simulations, because the computational power needed to invert the overlap operator, the time consuming part of the Hybrid Monte Carlo (HMC) algorithm, is too big.

In the past, we have been developing preconditioning and relaxation techniques which reduce the time needed for the inversion of the overlap operator by over a factor of 4, bringing the simulation of dynamical overlap fermions on medium-size lattices within the range of Teraflop computers.

In this paper we apply the HMC algorithm to overlap fermions. We approximate the matrix sign function using the Zolotarev rational approximation, treating the smallest eigenvalues of the Wilson operator exactly. We then derive the fermionic force for the overlap operator, presenting a new method for the treatment of zero crossings of the eigenmodes of the Wilson kernel. Our method, for the first time, is able to preserve the advantageous scaling of the Hybrid Monte Carlo algorithm.

Finally, we test our algorithm on small lattices with up to 12^4 sites at relatively small masses.

IC/MP199/020: Nonlinear eigenvalue problems.

Organiser: Heinrich Voss (TU Hamburg–Harburg, Germany)
Co-organiser: Elias Jarlebring (TU Braunschweig, Germany)

The nonlinear eigenvalue problem $T(\lambda)x = 0$, where $T : D \to \mathbb{C}^{n\times n}$ is a family of matrices depending on a parameter $\lambda \in D \subset \mathbb{C}$, arise in a wide variety of applications; e.g., sensitivity analysis of mechanical systems or micro electromechanical systems, vibrations of damped and/or rotating structures and of fluid–solid structures, the numerical simulation of semiconductor nano-structures and stability of time-delay systems and differential–difference equations.

The eight presentations of this minisymposium reflect some of the current challenges related to nonlinear eigenvalue problems and the pseudospectra of nonlinear eigenvalue problems. Systematic new linearization approaches for quadratic, and more generally polynomial eigenvalue problems are discussed that preserve internal structures such as eigenvalue symmetries. Minmax characterizations of real eigenvalues for some classes of problems are exploited for determining some extreme eigenpairs of large and sparse symmetric eigenproblems with applications to the Schrödinger equation depending rationally on the eigenparameter and to regularized total least squares problems. Two-sided Jacobi–Davidson type methods are proposed for computing eigenpairs of strongly non-Hermitean nonlinear problems, and are analyzed taking advantage of techniques from singularity theory. Structured pseudospectra are introduced for nonlinear eigenproblems including computable formulae, and are applied to the sensitivity analysis of eigenvalues of time-delay systems. Numerical methods to compute the spectrum of time-delay systems using rational interpolation are proposed, as well as some methods using pseudospectral approximations of partial retarded functional differential equations and its applications in robust control of time-delay systems.

Staircase forms and linearization of matrix polynomials. **Volker Mehrmann** (TU Berlin, Germany) IC/MT1174/020

The classical approach for the solution of nonlinear eigenvalue problems is linearization; i.e., the transformation to a larger linear eigenvalue problem. Unfortunately the classical companion forms destroy symmetry structures, while structured linearizations only work if certain eigenvalues are excluded in the original problem. We describe a new structured staircase form under unitary/orthogonal transformations for arbitrary matrix tuples and show how this can be used to determine structured linearizations.

Hyperbolic matrix polynomials and definite pencils. **D. Mackey** (Western Michigan University, USA) IC/MT2586/020

The usual definitions of definite pencil and hyperbolic quadratic polynomial make these two classes of matrix polynomial appear to be unrelated. However, it is well known that the corresponding eigenproblems have many properties in common; indeed, among matrix polynomial eigenproblems these can be regarded as the closest analogs of the standard eigenproblem for Hermitian matrices. In this talk we generalize the usual definition of hyperbolic polynomial, and see how this generalization both simplifies and unifies the notions of hyperbolic matrix polynomial and definite pencil. This connection is further strengthened by showing that a matrix polynomial is hyperbolic in this generalized sense if and only if it can be linearized by a definite pencil of a particular type.

This is joint work with Nicholas J. Higham and Françoise Tisseur of The University of Manchester, U.K.

A primal–dual Jacobi–Davidson-like method for nonlinear eigenvalue problems based on singularity theory. **Kathrin Schreiber** (TU Berlin, Germany), Hubert Schwetlick (TU Dresden, Germany) IC/MT1888/020

We present a Jacobi–Davidson like correction formula for left and right eigenvector approximations of strongly non-Hermitian nonlinear eigenvalue problems. It exploits techniques from singularity theory for characterizing singular points of nonlinear equations. Unlike standard nonlinear Jacobi–Davidson, the correction formula does not contain derivative information and works with orthogonal projectors only. Moreover, the basic method is modified in that the new eigenvalue approximation is taken as a nonlinear Rayleigh quotient obtained as root of a certain scalar nonlinear equation the existence of which is shown.

[1] Schwetlick, H. and Schreiber, K.; A primal-dual Jacobi–Davidson-like method for nonlinear eigenvalue problems. Internal Report ZIH-IR-0613, pp.1–20, Techn. Univ. Dresden, Zentrum für Informationsdienste und Hochleistungsrechnen, 2006. Submitted to *ETNA*.

Numerical simulation of the electronic structure of quantum dots. **Heinrich Voss** (TU Hamburg–Harburg, Germany) IC/MT1065/020

In semiconductor nanostructures free carriers are confined to a small region of space by potential barriers, and if the size of this region is less than the electron wavelength, the electronic states become quantized at discrete energy levels. The ultimate limit of low dimensional structures is the quantum dot, in which the carriers are confined in all three directions, thus reducing the degrees of freedom to zero.

The governing equation characterizing the relevant energy states λ and corresponding wave functions ψ is the Schrödinger equation

$$-\nabla\cdot\left(\frac{\hbar^2}{2m(\lambda)}\nabla\psi\right)+V\psi=\lambda\psi,$$

which depends nonlinearly on the eigenparameter if we assume a non-parabolic electron effective mass m.

Taking advantage of variational properties of the eigenproblem (which are inherited by finite element discretizations) it can be solved efficiently by iterative projection methods of Arnoldi or Jacobi-Davidson type combined with safeguarded iteration.

IC/MP199/020: Nonlinear eigenvalue problems. #2

Organiser: Heinrich Voss (TU Hamburg–Harburg, Germany)
Co-organiser: Elias Jarlebring (TU Braunschweig, Germany)

(For abstract, see session #1 above.)

Pseudo-spectra for nonlinear eigenvalue problems, with application to time-delay systems. **Wim Michiels** (Katholieke Universiteit Leuven, Belgium) IC/MT2509/020

In the first part of the presentation, various definitions for pseudospectra of a nonlinear eigenvalue problem are given, where the structure of the eigenvalue problem is exploited and, if needed, additional structure can be imposed on the matrices which occur in the definition of the eigenvalue problem. Various perturbation measures are considered and computationally tractable expressions are derived. The results are applied to classes of linear delay differential systems with uncertain coefficient matrices, whose transient behaviour and stability properties are determined by the solutions of a nonlinear eigenvalue problem. Special properties of the pseudospectra of such equations are discussed and illustrated.

In the second part of talk we address stability radii of stable linear time-delay systems, which can be defined as the size of smallest destabilizing perturbations. For time-invariant perturbations computational formulae can be directly obtained from the expressions for the pseusodpectra. Next, by taking an interconnection point of view and applying ideas from L2 gain analysis, we show how formulae for the stability radii can also be derived for the case where classes of time-varying perturbations are considered.

Examples from laser physics and structural dynamics will be used throughout the presentation, to illustrate the main ideas and results.

Rational interpolation iteration for eigenvalues of a delay-differential equation. **Elias Jarlebring** (TU Braunschweig, Germany) IC/MT1040/020

We present a new method to find the eigenvalues of a *single delay delay-differential equation*; i.e., the solutions $s\in C$ and $v\in C^n$ of the characteristic equation

$$\left(-sI+A_0+A_1e^{-\tau s}\right)v=0\,.$$

The method iteratively approximates the exponential term with a rational function, which is determined by selecting interpolation points at the eigenvalue-approximations of the previous iterate. The rational approximation of the characteristic equation is a *rational eigenvalue problem* and can be solved by known methods for such problems or be transformed to a *polynomial eigenproblem*. The convergence of the iteration is demonstrated with examples together with some conservative error-bounds. The advantages of the method are investigated by comparing it to standard methods for computing the eigenvalues of delay-differential equations.

Pseudo-spectral approximations of characteristic values of partial-retarded functional differential equations. **Dimitri Breda** (Università degli Studi di Udine, Italy), Stefano Maset (Università degli Studi di Trieste, Italy), Rossana Vermiglio (Università degli Studi di Udine, Italy) IC/MT2229/020

Partial differential equations of evolution involving time delay, also called Partial Retarded Functional Differential Equations (PRFDEs), arise in many fields: population ecology, control theory, genetic regression, climate models, structured population models.

In this talk we deal with semi-linear PRFDEs restated as abstract semi-linear RFDEs

$$\frac{du(t)}{dt} = A_T u(t) + F(u_t),\ t \geq 0,$$

where A_T is the infinitesimal generator of a strongly continuous semigroup of bounded linear operators on a complex Banach space X, $F : C \to X$ is a Lipschitz map defined on the space $C = C([-r, 0], X)$ with $r > 0$, and $u_t \in C$ is given by $u_t(\theta) = u(t + \theta)$, $\theta \in [-r, 0]$.

The stability analysis of equilibrium points plays a main role in the study of PRFDEs. It is well known that the asymptotic stability of an equilibrium point can be reduced to the asymptotic stability of the zero solution of the linear equation obtained by linearizing about the equilibrium point. The linearization of the semi-linear PRFDE about an equilibrium point yields the abstract fully-linear RFDE

$$\frac{du(t)}{dt} = A_T u(t) + L\,(u_t)\,,\ t \geq 0,$$

where $L : C \to X$ is a linear bounded operator.

Recently, several numerical approaches have been proposed to approximate the characteristic values of linear RFDEs, i.e. for X finite-dimensional and $A_T = 0$. One of these approaches consists in the discretization by a pseudospectral technique of the infinitesimal generator of the semigroup of the solution operators of the RFDE. In this talk such an approach is extended to the abstract fully-linear RFDE above.

On a quadratic eigen-problem occuring in regularized total least-squares. **Joerg Lampe** (TU Hamburg–Harburg, Germany), Heinrich Voss (TU Hamburg–Harburg, Germany) IC/MT1090/020

In a recent paper Sima, van Huffel and Golub suggested a computational approach for solving regularized total least squares problems via a sequence of quadratic eigenvalue problems. Taking advantage of a variational characterization of real eigenvalues of nonlinear eigenproblems we prove the existence of a right most eigenvalue. For large problems we improve the approach of Sima et al. considerably using thick and early updates in a Nonlinear Arnoldi method.

IC/MP76/020: Iterative solution of saddle-point systems arising in PDE-constrained optimization.

Organiser: Andy Wathen (University of Oxford, UK)
Co-organiser: Walter Zulehner (Universität Linz, Austria)

Significant improvements in computational power and the development of efficient algorithms for Partial Differential Equations (PDEs) have in the last several years enabled the solution of very large scale Optimization problems with PDE constraints; that is Optimization problems in which application of the constraints involves solving a PDE problem. Such problems give rise to sequences of very large dimensional linearized problems with the well-known saddle-point structure.

Preconditioned iterative approaches for the solution of these equations are the subject of this minisymposium.

Approximate nullspace iterations for KKT systems . **Volker Schulz** (Universität Trier, Germany) IC/MT1900/020

PDE constrained optimization problems lead naturally to Karush-Kuhn-Tucker (KKT) sytems, where the nullspace of the constraints is parameterized by the degrees of freedom for optimization. This nullspace cannot be computed exactly because this would mean the solution of many state PDEs. Therefore, classical Schur complement decomposition methods for KKT systems seem to be out of question. In this talk, novel convergence results are presented for approximate nullspace Schur complement decompositions used for the iterative solution of KKT systems. The importance of this research for practical applications is demonstrated in the field of shape optimization problems.

Multigrid solvers for very-large-scale saddle-point systems. **George Biros** (University of Pennsylvania, USA) IC/MT2796/020

In this talk we present multigrid smoothers for saddle-point Euler–Lagrange equations related to inverse problems for systems governed by parabolic PDEs. Due to the problem size of these problems, we have to devise matrix-free preconditioners. Due to the ill-conditioning, efficient multigrid solvers are required. The two key components of multigrid are the intergrid transfer operators, and the smoother. Here we restrict our attention to construction of efficient smoothers for full-space formulations of the inverse problem.

Preconditioners in optimal-control problems. **Ekkehard Sachs** (Universität Trier, Germany & Virginia Tech, USA) IC/MT3573/020

Optimal control problems with PDEs lead in discretized form to large scale optimization problems. Their numerical solution with SQP methods or interior point problems often requires the solution of saddle point problems as subproblems per iteration. The choice of appropriate preconditioners for an iterative solver is important for the efficiency of the method.

We review in particular the conjugate gradient method, which is especially suitable for optimization problems and investigate the infinite dimensional setting and its consequences for finite dimensional approximations.

A block-diagonal preconditioner for a saddle-point formulation of the Maxwell equations. **Chen Greif** (University of British Columbia, Canada) IC/MT1646/020

We discuss block preconditioning techniques for iteratively solving linear systems arising from finite element discretizations of the mixed formulation of the time-harmonic Maxwell equations. The preconditioners are motivated by spectral equivalence properties of the discrete operators, but are augmentation-free and Schur complement-free. We provide a complete spectral analysis, and show that the eigenvalues of the preconditioned matrix are strongly clustered. We show that the scalar Laplacian can be used as a weight matrix, and augmented terms can be replaced by matrices that are easier to solve for. Inexact solves based on the theory of inner/outer iterations further reduce the computational cost of the solver. An efficient implementation based on multigrid in a parallel computing environment deomonstrates the scalability of proposed approach.

IC/MP214/020: Multiscale porous media: solvers.

Organiser: Mary Wheeler (University of Texas at Austin, USA)
Co-organiser: Ivan Graham (University of Bath, UK)
Co-organiser: Robert Scheichl (University of Bath, UK)

Multiphase flow, transport, and reaction in porous media have important applications in petroleum reservoir engineering and in groundwater flow. These often involve multiphase multiphysics processes across multiple temporal and spatial scales whose discretisation leads to large highly ill-conditioned linear systems. This minisymposium showcases recent advances in solvers for these systems, with emphasis on special domain decomposition, multilevel and deflation methods. It is linked to the two other minisymposia: "Multiscale porous media: discretizations" and "Multiscale porous media: applications"

Domain decomposition methods for multiscale elliptic PDEs. **Ivan Graham** (University of Bath, UK) IC/MT1739/020

In this talk we will discuss domain decomposition preconditioning for linear systems arising from finite element approximation of symmetric elliptic problems with highly variable coefficients. The work is motivated by problems arising in the computation of flow through heterogeneous media. We will give condition number bounds which demonstrate how the subdomains and coarse space basis functions should be designed in order for the methods to be robust to both the heterogeneity of the media and the mesh parameters. In particular, we give a rigorous connection between low energy basis functions and robustness to heterogeneity. The results are illustrated by examples showing the benefits of using multiscale finite element interpolation as a coarsener.

Robust coarsening for multiscale PDEs. **Robert Scheichl** (University of Bath, UK) IC/MT1735/020

We consider two-level overlapping domain decomposition preconditioners for piecewise linear finite element approximations of elliptic PDEs with highly variable coefficients, as they arise in practice, for example, in the computation of flows in heterogeneous porous media, in both the deterministic and (Monte-Carlo simulated) stochastic cases. We propose and analyse new robust coarsening strategies for these problems, e.g. based on smoothed aggregation and multiscale finite elements, and study different ways of combining the coarse solve with the local solves (i.e. additive, multiplicative and deflation). We will use and extend a recently developed general framework for analysing the resulting preconditioners to show their robustness for a variety of model situations, but we will also focus in this talk on linear algebra and parallelisation aspects. Numerical experiments will be used to illustrate the robustness and efficiency of the proposed methods and the sharpness of our theoretical results.

This is joint work with I.G. Graham and J. Van lent (University of Bath) and E. Vainikko (University of Tartu, Estonia).

Multiscale deflation solvers for flow in porous media. **Hector Klie** (University of Texas at Austin, USA), Adolfo Rodriguez (University of Texas at Austin, USA), Mary Wheeler (University of Texas at Austin, USA) IC/MT1613/020

It is a well-known fact that the ill-conditioning of linear systems arising in porous media flow applications is mainly due to the high variability and poor correlation lengths shown by most realistic permeability/porosity field distributions. This fact has been one of the main factors limiting the applicability of standard algebraic solutions for a wide range of linear systems arising in many fluid flow simulations. This work describes a novel physics-based deflation preconditioner approach for solving porous media flow problems characterized by highly heterogeneous media. The approach relies on fast-flow block solutions after rearranging the linear system coefficients into a fast-flow and slow-flow blocks from a given physically driven threshold value. This rearranging may either follow a static inspection of the permeability field or follow flow field information obtained from a lower complexity flow model (e.g., single phase-flow or streamline simulator). Hence, the preconditioner strategy is built upon the premise that flow trends (driven by the connectivity of high permeability regions) should determine the relevance of the coefficient blocks to be included in the solution process. The resulting preconditioner may alternatively be combined with a Krylov-based or domain-based deflation preconditioning stage. This additional operation allows for the removal of the negative effect that extreme (usually small) eigenvalues may have on the convergence of the Krylov iterative method. Generally, these extreme eigenvalues are associated with unresolved error frequencies due to local permeability contrasts and small flow contributions from low-permeability regions. The proposed approach is labeled as a physics-based 2-stage, deflation preconditioner (P2SDP). Numerical experiments on different permeability distributions reveal that the P2SDP is a powerful means to solve pressure systems when compared to more conventional algebraic approaches such as ILU and block preconditioners.

Projection acceleration of Krylov solvers. **Cornelis Vuik** (TU Delft, The Netherlands) IC/MT1847/020

To predict the presence of oil and natural gas in a reservoir it is important to know the fluid pressure in the rock formations. A mathematical model for the prediction of fluid pressure is given by a time-dependent diffusion equation. Application of the finite element method leads to systems of linear equations. A complication is that the underground consists of layers with very large contrasts in permeability. This implies that the symmetric and positive definite coefficient matrix has a very large condition number. Bad convergence behavior of the ICCG method has been observed, and a classical termination criterion is not valid in this problem.

Other applications, where the coefficients have large discontinuities are electrical power networks, groundwater flow, semiconductors, and electromagnetic modeling.

In this paper it is proven that the number of small eigenvalues of the IC preconditioned matrix is equal to the number of high permeable domains, which are not connected to a Dirichlet boundary. It appears that the Deflated ICCG method annihilates the effect of these small eigenvalues. A method is given to construct the corresponding projection vectors in an efficient way. Furthermore it is proven that the span of these vectors is close to the 'small' eigenspace. A theoretical investigation and numerical experiments show that the DICCG method is not sensitive to small perturbations of the projection vectors. The efficiency of the DICCG method is illustrated by numerical experiments.

Problems with large jumps in the coefficients can also be solved with a suitable (additive) coarse grid correction. In this paper we compare deflation with the additive coarse grid correction and the balancing preconditioner.

IC/MP98/021: Algorithms for high-dimensional problems.

Organiser: Josef Dick (UNSW Asia, Singapore)
Co-organiser: Frances Kuo (University of New South Wales, Australia)

Applications often require concrete algorithms for solving high dimensional problems like numerical integration, approximation, function recovery, maximum likelihood estimation, solving integral equations, pde's, sde's and so on, to name but a few.

In this double session some of the leading researchers in the field will present their newest research concerning the analysis and/or implementation of algorithms which can be used for solving some high dimensional problems.

Sparse grids for the approximation of probability densities. **Markus Hegland** (Australian National University) IC/MT1488/021

Probability densities are widely used in statistics, machine learning and stochastic modelling. They provide a tool for exploring features like clusters and moments of populations of objects. Traditional statistical techniques include histograms, kernel density estimators and (penalised) maximum likelihood methods. They all face the classical dilemma when applied to high-dimensional data: either the complexity is exponential in the dimension as in the example of histograms or the evaluation complexity is proportional to the number of data points as in the example of kernel density estimators.

Here we will discuss inference methods for (conditional) densities using stochastic process priors and several divergences. Furthermore we will introduce new graphical models based sparse grids for density approximation.

Optimal algorithms for approximation of piecewise r-smooth functions. **Leszek Plaskota** (Uniwersytet Warszawski, Poland) IC/MT4981/021

We study optimal algorithms for approximating functions (pictures) that are piecewise r-smooth, in the worst case and asymptotic settings. Traditional (nonadaptive) methods that are optimal for globally r-smooth functions are generally useless in this case. Hence one has to switch to adaptive methods to achieve best possible convergence rate, which is n^{-r} where n is the number of function evaluations.

The obtained results are very much sensitive to the metric in which the error of approximation is measured. For instance, there are no algorithms with uniform error converging to zero for discontinuous functions. If the error is meaured in the Skorohod metric (which is roughly the uniform distance between the original and slightly perturbed pictures) then there are adaptive algorithms with error n^{-r}. Similar positive results can be obtained even in the uniform norm if the functions under consideration are globally continuous.

The optimal algorithms generally use interpolation/extrapolation methods that are based on adaptively chosen samples.

On the convergence of quasi-random sampling importance resampling. **Ronald Cools** (Katholieke Universiteit Leuven, Belgium), Bart Vandewoestyne (Katholieke Universiteit Leuven, Belgium) IC/MT943/021

In this talk, we discuss the problem of generating representative point sets from a distribution known up to a multiplicative constant. The Sampling/Importance Resampling (SIR) algorithm is known to be useful in this context. The Quasi-random Sampling Importance Resampling (QSIR) scheme, based on quasi-Monte Carlo methods, is a recent modification of the SIR algorithm and was empirically shown to have a better rate of convergence. Exploiting the theory of quasi-Monte Carlo and restricting ourselves to distributions with independent and identically distributed marginals, we construct asymptotic error bounds for the QSIR scheme.

Strong tractability of multivariate integration of arbitrary high order using polynomial lattice rules. **Friedrich Pillichshammer** (Universität Linz, Austria), Josef Dick (UNSW Asia, Singapore) IC/MT989/015

We show the existence of digitally-shifted polynomial lattice rules which achieve strong tractability results for Sobolev spaces of arbitrary high smoothness. The convergence rate is shown to be best possible up to a given degree of smoothness of the integrand.

IC/MP98/021: Algorithms for high-dimensional problems. #2

Organiser: Josef Dick (UNSW Asia, Singapore)
Co-organiser: Frances Kuo (University of New South Wales, Australia)

(For abstract, see session #1 above.)

Lower-dimensional manifold detection in high-dimensional data spaces by dimension-adaptive sparse grids. **Michael Griebel** (Universität Bonn, Germany) IC/MT1332/021

High-dimensional problems and data often live in a lower-dimensional subspace or manifold with relatively small intrinsic dimension. In such cases it is possible to break the curse of dimensionality, i.e. to circumvent the exponential dependency on the high dimension in the complexity of associated algorithms, by transferring the problem approximatively into a representation which uses the intrinsic coordinates of the lower-dimensional subspace. We then may design algorithms whose complexity only depend (exponentially) on the dimension of this subspace. Unfortunately, neither the lower-dimensional subspace/manifold nor its (non-linear) coordinate system is usually known a-priori.

We discuss how such lower-dimensional manifolds can be detected by dimension-adaptive sparse grid methods.

Randomized Smolyak algorithms based on digital sequences for multivariate integration. **Gunther Leobacher** (Universität Linz, Austria), Friedrich Pillichshammer (Universität Linz, Austria), Josef Dick (UNSW Asia, Singapore) IC/MT1157/021

In this paper we consider Smolyak algorithms for high dimensional numerical integration. The quadrature rules are equal weight quadrature rules based on digital $(t, \alpha, \beta, \sigma, d)$-sequences. As those sequences can be randomized we obtain a randomized Smolyak algorithm. We consider the worst-case error in certain Sobolev spaces and show that our quadrature rules achieve the optimal rate of convergence. This result holds for the randomized as well as for the deterministic algorithm. We also show that the randomized algorithm is unbiased and that the integration error can be approximated as well.

Quasi-Monte-Carlo for Markov chain Monte-Carlo. **Art Owen** (Stanford University, USA) IC/MT970/021

There has been considerable progress recently in developing improvements to Monte Carlo methods. Quasi-Monte Carlo (QMC) methods improve MC accuracy by using a more balanced sampling. Markov chain Monte Carlo (MCMC) widens the applicability of MC to problems where we cannot sample IID from the desired distribution. The published intersection between these two methods is conspicuously small.

To use QMC points in the MCMC context, one seeks to achieve equidistribution in $[0,1]^\infty$. We show that some but not all QMC points give rise to consistent estimates in Metropolis-Hastings algorithms, including the Gibbs sampler. The suitable points are completely uniformly distributed (CUD). In some numerical examples, variance reduction factors seen range from just over 2 to just over 240. The Gibbs sampler seems to be well suited to QMC inputs.

This is joint work with Seth Tribble.

Finite-order lattice rules can be dangerous. **Ian Sloan** (University of New South Wales, Australia) IC/MT949/021

Lattice rules constructed by the component-by-component algorithm are known to provide an effective approximation scheme for many high-dimensional problems formulated as integrals over the d-dimensional unit cube. In this talk it is demonstrated that the use of so-called finite-order weights can be dangerous for applications. The danger lies in the fact that a lattice rule constructed with say order-2 weights can have very bad 3-dimensional projections. As a result, if the integrand cannot be expressed exactly as the sum of functions of two variables at a time then there is no guarantee of convergence as the number of integration points approaches ∞.

IC/MP330/021: Approximate algebraic methods for computer-aided geometric design.

Organiser: Tor Dokken (SINTEF, Norway)

Although the origin of algebraic geometry was to solve geometric problems of daily life, current research is addressing problems described in homogeneous coordinates and complex spaces. The introduction of computers more than five decades ago triggered research in Computer Aided Geometric Design (CAGD). This research has always been focused on what is feasible to compute on available commodity computers. The continuous increase in computational performance has also triggered demands for better quality and higher accuracy in Computer Aided Design systems, especially with respect to surface intersection algorithms.

To try to satisfy these demands researchers in classical Algebraic Geometry and researches in CAGD have in recent years joined forces to address challenges related to geometry representation and interrogation in producing industries. The EU IST-2001-35512 project *Intersection algorithms for geometry based IT-applications using approximate algebraic methods* addressed the problems of problematic intersections in CAD-systems. The focus was surface self-intersections and situations where surfaces are near parallel in intervals along the intersection curves. The project addressed the challenges from the viewpoint of exact computations, semi-numeric computations and a numeric recursive subdivision approach. After the project end the project partners have continued their research. The mini-symposium will focus on experiences of such a focused research project and results from and after the project. It will address:

- approximate implicitization, how to approximate parametric surfaces by real algebraic surfaces;
- exact, numeric and recursive intersection algorithms;
- resolving topological questions in practice about real curves and surfaces;
- use of multi-core CPUs and programmable graphics cards for improving quality and performance of intersection algorithms.

The use of approximate implicitization in recursive surface-intersection algorithm. **Tor Dokken** (SINTEF, Norway) IC/MT1331/021

Most published work on NURBS surface intersection address *transversal intersections*, situations where the surface normals of the surfaces interesected are well separated along all intersection curves. NURBS - NonUniform Rational B-splines is the standard representation for parametric surfaces in CAD. For transversal intersections the divide and conquer strategy of recursive subdivision, Sinha's theorem and the convex hull property of NURBS surfaces efficiently identify all intersection branches. However, in *singular or near singular intersections*, situations where the surfaces are parallel or near parallel in an intersection region, along an intersection curve or in an intersection point, even deep levels of subdivision will frequently not sort out the intersection topology.

The talk will focus on two novel approaches to address this situation:

- Use of *approximate implicitization* for separation of near parallel curves or surfaces, and for detecting a monotone relation between two curves or two surfaces. Approximate implicitization denotes methods that within a region of interest approximate a parametric curve or surface with respectively an real algebraic curve or surface of lower degree than the exact algebraic representation.
- Use of parallel processing on multi-core CPUs or programmable graphic cards (GPUs) to establish when the intersection is transversal, and when the intersection is singular or near singular. Many standard GPUs have currently one to two orders of magnitude higher computational performance than a single-core CPU. Such performance can be used for simplistic subdivision of surfaces to detect intersections that are clearly transversal and identify intersections that possibly are singular or near singular.

Gauss–Newton-type techniques for l^p approximation. **Martin Aigner** (Universität Linz, Austria), Bert Juttler (Universität Linz, Austria) IC/MT1846/021

We consider the problem of fitting a parametric or implicitly defined curve or surface to given scattered data. In order to minimize the influence of noise and of outliers, it is desirable to consider the l^p norm of the error vector for small values of p (p≥1). On the other hand, in order to minimize the maximum error, it is useful to consider l^p norms for large values of p. In this talk we derive Gauss-Newton-type techniques for minimizing these l^p norms and analyze their relation to the method of iteratively reweighted least-squares fitting.

Mixing symbolic and numerical approaches for the surface-to-surface intersection problem. **Mario Fioravanti** (Universidad de Cantabria, Spain), Laureano Gonzalez-Vega (Universidad de Cantabria, Spain) IC/MT2019/021

The Surface-to-Surface Intersection Problem is one of the most critical tasks in Computer Aided Geometric Design. In this talk it will be shown how the efficiency of current methodologies dealing with this problem can be improved by combining an algebraic/symbolic framework with efficient and robust numerical techniques.

The algebraic/symbolic framework will be used to translate the computation of resultants, subresultants, discriminants, etc. (needed when approaching this problem symbolically) to one or several generalized eigenvalue problems and SVD computations. The framework requires only the values of the involved polynomial at some set of points (i.e. the monomial description of them may not be available). This framework will guide the numerical solving of the above mentioned problems providing thus a certificate of the topological correctness of the output.

As particular cases, the following problems will be also shown to be solved by using this approach:

- Computing the topology of $f(x,y)=0$.
- Computing the topology of the offset of $f(x,y)=0$ to distance d.
- Computing the intersection points between the offsets of planar parametric curves.

Symbolic–numeric methods for semi-algebraic shapes. **Bernard Mourrain** (INRIA Rocquencourt, France) IC/MT2104/021

We are interested by shapes represented by semi-algebraic models, such as parameterized curves and surfaces which are the basis of classical geometric modeler, but also by implicit representations, which allows compact and powerful representations of geometric objects. Performing geometric operations on these models require on one hand topological computation and on the other hand numerical approximation. In particular, it leads to the manipulation of roots of polynomial equations. We are going to detail methods which exploit a duality between exact implicit and approximate computation in these problems and show how to combine for analysing singularities of such objects or computing their topology, (self)-intersection curves. We will illustrate it by some experiments with the library SYNAPS, integrated in the modeler AXEL.

IC/MP1067/021: Sparse grids for high-dimensional approximation.

Organiser: Michael Griebel (Universität Bonn, Germany)
Co-organiser: Markus Hegland (Australian National University)
Co-organiser: Christoph Schwab (ETH Zürich, Switzerland)

Sparse grids are a special discretization technique for the approximation of high-dimensional functions. Based on a sparse tensor product construction they employ only $O(N(\log N)^{d-1})$ grid points, where N denotes the number of points in one dimension and d the number of dimensions. The achieved accuracy is nearly the same as the one obtained on conventional uniform grids provided that the smoothness assumption of bounded mixed derivatives is fulfilled. Thus sparse grids allow to cope with the curse of dimensionality of grid based approaches to a certain extent. The minisymposium will present an overview of the approach with an emphasis on recent developments in the theory of the sparse grid combination technique and on applications of sparse grids for the solution of high-dimensional partial differential equations and in machine learning.

Deterministic simulation for asset–liability management in life insurance. **Markus Holtz** (Universität Bonn, Germany) IC/MT3824/021

New regulations and a stronger competition have increased the importance of stochastic asset-liability-management models for insurance companies in recent years. In this talk, we propose deterministic integration schemes for the simulation of such models, such as quasi-Monte Carlo and sparse grid methods. Numerical examples demonstrate that these deterministic methods outperform Monte Carlo simulation even for long time horizons. The success of the deterministic integration schemes can be explained using the concept of the effective dimension and the concentration of measure phenomenon. Further efficiency improvements are achieved by dimension-adaptive sparse grid algorithms as we finally demonstrate by numerical examples.

Sparse finite elements for radiative transfer. **Gisela Widmer** (ETH Zürich, Switzerland), Ralf Hiptmair (ETH Zürich, Switzerland), Christoph Schwab (ETH Zürich, Switzerland) IC/MT3879/021

The linear radiative transfer equation, a partial differential equation for the intensity $u(\mathbf{x},\mathbf{s})$, with independent variables $\mathbf{x}\in D\subset\mathbb{R}^n$, $n=2,3$ and ß $\in S^2:=\{\mathbf{y}\in\mathbb{R}^3:|\mathbf{y}|=1\}$, is considered in the $n+2$-dimensional tensor product domain $D\times S^2$.

We propose and analyse an adaptive multilevel Galerkin FEM for the efficient numerical solution of the radiative transfer equation. Our method is based on: a) a stabilized variational formulation, and on b) so-called sparse tensor products of two hierarchic families of Finite Element spaces in $H^1(D)$ and in $L^2(S^2)$, respectively.

Specifically, we use wavelet decompositions of Finite Element spaces of continuous, piecewise linear functions on simplicial triangulations of the physical domain D and of discontinuous, piecewise constants on S^2.

We describe the details of the sparse tensor product spaces with adaptive, anisotropic mesh refinements in $D\times S^2$. A convergence analysis under strong regularity assumptions on the solution shows that the method converges with essentially optimal asymptotic rates while its complexity grows essentially only as that for a linear transport problem in $\mathbb{R}^n$. Numerical experiments for $n=2$ agree with the convergence and complexity analysis of the method and show its performance to be superior to the discrete ordinate method.

Sparse finite element approximation of high-dimensional transport-dominated diffusion problems. **Endre Süli** (University of Oxford, UK), Christoph Schwab (ETH Zürich, Switzerland), Radu-Alexandru Todor (ETH Zürich, Switzerland) IC/MT4954/021

Partial differential equations with nonnegative characteristic form arise in numerous mathematical models in science. In problems of this kind, the exponential growth of computational complexity as a function of the dimension d of the problem domain, the so-called "curse of dimension", is exacerbated by the fact that the problem may be transport-dominated.

We develop the numerical analysis of stabilized sparse tensor product finite element methods for such high-dimensional, non-self-adjoint and possibly degenerate second-order partial differential equations, using piecewise polynomials of degree $p\geq 1$. Our convergence analysis is based on new high-dimensional approximation results in sparse tensor-product spaces. By tracking the dependence of the various constants on the dimension d and the polynomial degree p, we show in the case of elliptic transport-dominated diffusion problems that for $p\geq 1$ the error-constant exhibits exponential decay

as $d \to \infty$. In the general case when the characteristic form of the partial differential equation is non-negative, under a mild condition relating p to d, the error constant is shown to grow no faster than $\mathcal{O}(d^2)$. In any case, the sparse stabilized finite element method exhibits an optimal rate of convergence with respect to the mesh size h_L, up to a factor that is polylogarithmic in h_L.

The talk is based on a recent paper available from: http://web.comlab.ox.ac.uk/oucl/publications/natr/NA-07-04.html.

Probability-density estimation using sparse grids. **Stephen Roberts** (Australian National University) IC/MT2830/021

In this talk we will discuss the use of sparse grid spaces for the estimation of high dimensional probability density functions. We will consider histosplines, L^2 projections and simple direct estimates via the cumulative distribution function. We investigate the convergence properties of these methods and show, for instance, that for a smooth enough underlying probability density function, the approximation error is $\log(N)^{d-1}N^{-2}$, where N is the dimension of the underlying sparse grid approximating space. The use of classical sparse grids allows us to practically deal with data sets with up to 15 dimensions. The methods are demonstrated on a 10 dimensional data collection containing information on vegetation cover and various geographical features.

IC/MP1067/021: Sparse grids for high-dimensional approximation. #2

Organiser: Michael Griebel (Universität Bonn, Germany)
Co-organiser: Markus Hegland (Australian National University)
Co-organiser: Christoph Schwab (ETH Zürich, Switzerland)

(For abstract, see session #1 above.)

Stochastic Galerkin method with sparse polynomial-chaos expansion. **Marcel Bieri** (ETH Zürich, Switzerland), Christoph Schwab (ETH Zürich, Switzerland) IC/MT1304/021

We consider a deterministic finite element (FE) solution algorithm for solving stochastic elliptic boudary value problems of the form

$$\begin{cases} -\mathrm{div}(a(x,\omega)\nabla u(x,\omega)) = f(x) & \text{in } D,\ u(x,\omega)|_{x\in\partial D} = 0, \quad P\text{-a.e. } \omega\in\Omega. \end{cases}$$

A separation of deterministic and stochastic variables is achieved via a Karhunen-Loève expansion, which leads to a high-dimensional but now purely deterministic problem. To overcome this high complexity we propose a sparse polynomial chaos expansion (SPC) to handle the stochastic parameters whereas for the spatial part a generic FE-solver can be used. Mathematical as well as numerical results will be presented to show convergence rates of the proposed algorithm.

An optimised sparse grid combination technique for eigenvalue problems. **Jochen Garcke** (TU Berlin, Germany) IC/MT1893/021

Recently an optimised combination technique for regression applications in machine learning was introduced. The original combination technique employs solutions on a certain sequence of (small) grids, a sparse grid solution is then obtained by addition of these partial solutions with combination coefficients which depend on the involved grids. For regression this approach shows instabilities in certain situations and is not guaranteed to converge with higher discretisation levels. In the case of the optimised combination technique the coefficients also depend on the function to be representend, a nonlinear approach, with this approach these instabilities disappear. In this talk I will show how to transfer the idea of an optimised sparse grid combination technique to eigenvalue problems. Besides the potential for improved accuracies the optimised combination coefficients also simplify the normalisation of the partial eigenfunctions. This arises since only the eigenspace is clearly defined, i.e. the partial eigenfunction have to be normalised to able to be combined in a suitable way, the optimised combination coefficients automatically take care of this issue. Numerical results for the Schrödinger equation in the case of hydrogen (in 3 space dimensions) and helium (in 6 space dimensions) are shown.

An efficient sparse-grid method for the high-dimensional Fokker–Planck equation. **Christian Feuers** (Universität Bonn, Germany) IC/MT2731/021

Numerical methods to solve the high-dimensional Fokker–Planck-equation are limited by the so called *curse of dimension'*, which restricts applications to three, maybe four space dimensions. We propose a sparse grid method for higher dimensions in order to benefit from the reduced grid complexity $O(N\log^{d-1}N)$ instead of $O(N^d)$ for classical methods. We employ timestepping schemes with variable step-size control in time and a sparse grid galerkin method in space for each time step. New matrix–vector-product algorithms for the semi-orthogonal prewavelet basis reduce the typically required 2^d grid traversals to just a constant number. We present efficient hash-based storage techniques which allow to solve the linear systems without influence of the dimension to storage requirements. While the number of iterations is known to be independend of the mesh width, its dependence on the problem dimension is discussed based on numerical experiments. The accuracy of the method is analysed by means of higher dimensional model problems. Finally, we apply the method to stochastic models in finance and present numerical results.

The combination technique and some generalisations. **Markus Hegland** (Australian National University), Jochen Garcke (TU Berlin, Germany) IC/MT4955/021

Sparse grids often effectively address the curse of dimensionality. When solving the equations for sparse grid approximations, however, one has to solve linear systems of equations which lack the typical banded or block structure which reflects the symmetry of regular grids. It has been found in the past that simple combinations of solutions on regular subgrids of a sparse grid frequently provide a good approximations to sparse grid solutions. These combinations are exact for interpolation problems, have been shown to lead to an extrapolation technique for the Poisson problem but they can also fail spectacularly, especially when applied in high-dimensional situations for adaptive sparse grids.

In the talk I will discuss an analysis of the combination technique using a projection framework and the C/S decomposition. This analysis provides connections between geometric properties and the errors of the combination technique. It will be seen how the combination technique can be improved, and we will in particular discuss the Opticom technique which uses optimal combination coefficients which are adapted to the problem and data.

This is joint work with Jochen Garcke and Vivien Challis.

IC/MP137/022: Multivariate numerical integration.

Organiser: Ronald Cools (Katholieke Universiteit Leuven, Belgium)

Integrals appear in many mathematical models and can seldom be calculated analytically. The numerical approximation of integrals is therefore one of the corner stones of numerical analysis. As computers become more powerful every day, researchers start thinking about problems nobody dreamed about some years ago, resulting in e.g. integrals with hundreds of variables.

In this minisymposium we will focus on recent developments in this area, ranging from new approaches for the construction of basic integration rules (cubature formulas) to techniques that are tailored to the application.

A cardinal function algorithm for computing cubature points. **Mark Taylor** (Sandia National Laboratories, USA) IC/MT1766/022

An effective method for constructing quadrature and cubature formulas is to numerically solve a nonlinear set of equations for the quadrature points and their associated weights. Newton's method is often used, combined with symmetry conditions to reduce the number of equations and unknowns. Here we present two improvements to this approach: We write the equations using a cardinal function basis which allows us to treat the quadrature weights as dependent variables and remove them, as well as an equivalent number of equations, from the numerical optimization procedure. Then, in the triangle, we construct initial conditions for Newton's method which approximate the pluri-potential theory extremal measure. We give results for the triangle, where for all degree $d \leq 25$, we find quadrature formulas which have positive weights and contain no points outside the triangle. Seven of these quadrature formulas improve on previously known results.

We also use this algorithm to construct cubature formulas specialized for a high-order mass-lumped finite element method (Cohen, Joly and Tordjman, 1995) This method requires cubature formulas with strength $2d$ to have $3d$ points along the boundary. Such formulas have previously been computed up to $d = 5$ (Mulder, 2000) and we extend these results to $d = 6, 7$.

elrint3d: an automatic 3D cubature routine. **Ian Robinson** (La Trobe University, Australia) IC/MT1631/022

We describe an automatic algorithm for three-dimensional cubature over quite general regions that is non-adaptive and based on an embedded lattice augmentation sequence. The algorithm is shown to be extremely efficient and effective for a wide range of functions, including smooth functions and functions with singularities at a vertex or along a boundary of the integration region.

Adaptive quasi-Monte Carlo methods for fast evaluation of contingent claims. **Ben Waterhouse** (University of New South Wales, Australia) IC/MT1489/022

The area of numerical integration is of great interest to practitioners of mathematical finance. Many integration problems encountered in mathematical finance involve integrands which are constant for large regions of the domain. This is common for derivatives which are *rare*, such as an out-of-the-money call option with a high strike price, or a digital option which is constant almost everywhere. MC and QMC methods are blind to the pay-off function and will sample throughout the domain. We would like to create methods which sample adaptively and which seek out the *interesting* regions of most variation first.

For the MC approach there are methods such as stratified sampling which will find the regions which are most important. These approaches often become much less attractive as the *curse of dimensionality* sets in.

For QMC methods, comparatively little has been done in the area of adaptive sampling. The work of Dahl proposed an adaptive algorithm for evaluation of contingent claims however it did not outperform traditional QMC methods for problems of moderate dimension. The work of Schuerer applied the ideas of the MISER and VEGAS algorithms for MC points to the QMC points. The results in this paper showed that the adaptive algorithm was beneficial for problems with dimension up to 5.

In this talk, we propose a similar algorithm which exploits the observation that many high-dimensional integrands can be written as integrands with low effective dimension. This means that we need not adaptively sample over all dimensions, but rather only those few which are of most importance. We see that by exploiting the net properties of Sobol' points and other (t, m, s)-nets, we may achieve improvements in convergence of an order of magnitude or more over traditional QMC methods. Moreover, it can be used for problems with a nominal dimension in the hundreds or higher.

Computation of Feynman loop integrals. **Elise de Doncker** (Western Michigan University, USA) IC/MT3594/022

We include a survey of the authors' and related work on multivariate integration and extrapolation techniques for the computation of Feynman loop integrals. Loop integrals are required for perturbation calculations in high energy physics, as they contribute corrections to the scattering amplitude and the cross section for the collision of elementary particles.

The term "loop" refers to the occurrence of one or multiple loops in the corresponding Feynman diagrams. In earlier work we studied the application of extrapolation based techniques to the computation of one-loop three-point (vertex) and four-point (box) diagrams, and two-loop planar (ladder) vertex diagrams. We will furthermore present more recent results for two-loop non-planar (crossed) vertex diagrams.

The integrals are particularly difficult as the integrand generally exhibits a singularity within the integration domain. The integral approximation is obtained in the limit as the value of a parameter, epsilon, in the integrand tends to zero. This involves the numerical evaluation of a sequence of integrals for decreasing epsilon, and a procedure for convergence acceleration.

We use "iterated" integration to calculate the multivariate integrals. Various one- and multi-dimensional integration methods can be combined and used in different sets of coordinate directions. We found that standard multi-dimensional integration techniques do not deliver the required results for this application. The combined integration and extrapolation methods aim for an automatic calculation, where little or no analytic manipulation is required before the numeric approximation.

This work is performed in cooperation with: Y. Shimizu (Grad. Univ. for Advanced Studies, Hayama, Japan); J. Fujimoto, T. Ishikawa and F. Yuasa (High Energy Accelerator Research Organization, Tsukuba, Japan); N. Hamaguchi (Hitachi, Ltd., Software Division, Totsuka-ku, Yokohama, Japan).

IC/MP96/022: Modern constructions of low-discrepancy sequences.

Organiser: Friedrich Pillichshammer (Universität Linz, Austria)
Co-organiser: Peter Kritzer (Universität Salzburg, Austria)

In many applications, notably quasi-Monte Carlo integration, point sets in the high dimensional unit cube with excellent distribution properties are required. A common measure for the quality of the distribution of a point set is the so-called discrepancy. Informally one will call a point set a low discrepancy point set if its discrepancy is of order $O((\log N)^s/N)$, where N is the cardinality of the point set and s is the dimension.This two-session minisymposium considers the construction and analysis of low discrepancy sequences, such as digital nets, lattice point sets and others. Furthermore, different measures of the quality of distribution of low discrepancy point sets are analyzed.

This minisymposium is closely related to the minisymposia "Algorithms for high dimensional problems" and "Complexity of high dimensional problems".

On the L_2-discrepancy of van der Corput sequences. **Henri Faure** (Université de la Méditerrannée Aix-Marseille II, France) IC/MT1013/0

Van der Corput sequences in arbitrary bases are the prototype for the construction of low discrepancy sequences widely used in numerical integration and quasi-Monte Carlo methods. Many people in the last few years have paid great attention to the behaviour of different generalizations of van der Corput sequences, especially in base two. In this communication, we will present a survey of the previous results concerning the L_2-discrepancy and then, we will introduce a method which allows to recover some results in base two and to generalize them to other bases. Hopefully, the method should also provide the answer to a recent conjecture on the L_2-discrepancy of shifted van der Corput sequences in base two (Kritzer-Pillichshammer, 2005).

Construction of digital nets based on propagation rules for OOAs. **Rudolf Schürer** (Universität Salzburg, Austria) IC/MT1195/0

(t,m,s)-*nets* are a powerful tool for the generation of low-discrepancy point sets. Based on the digit expansion of the points of a net an equivalent combinatorial object can be obtained, namely a certain subclass of an *ordered orthogonal array* (*OOA*).

Many constructions and propagation rules for nets can alternatively be formulated in the language of OOAs. In this setting it becomes apparent that these methods match well-known constructions for *orthogonal arrays* (*OAs*), which are the special case of OOAs with depth $T = 1$, whereas nets correspond to the case with depth T equal to the strength k of the OOA.

Most previous work focuses either on nets, OAs, or on obtaining a net directly from an OA. We discuss new constructions of nets that are based on OOAs with a depth strictly between 1 and k. Using a combination of such methods we obtain new nets with parameters superior to earlier results.

On linear-programming bounds for nets. **Horst Trinker** (Universität Salzburg, Austria), Wolfgang Schmid (Universität Salzburg, Austria) IC/MT1556/0

It is well known that there are close connections between low-discrepancy point sets and sequences at the one side and certain combinatorial and algebraic structures at the other side. E.g., Niederreiter (1992) showed the equivalence between $(t,t+2,s)$-nets and orthogonal arrays (OAs) of strength 2. Some years later this was generalized and made precise in the work of Lawrence, Mullen, and Schmid by introducing ordered orthogonal arrays (OOAs). This large class of combinatorial structures yields both new constructions and bounds for the existence of nets and sequences.

As in the case of linear codes and OAs, the linear programming (LP) bound is a very strong bound for OOAs and consequently for nets and sequences. The LP bound for OOAs was first derived by Martin and Stinson (1999).

Calculating LP bounds on OAs and OOAs in exact arithmetic is very time-consuming. We have studied different approaches for reducing the computing time and will give a survey of our results.

For OAs in basis $q = 2$ Bierbrauer et al. (1999) have shown that the dual Plotkin bound is optimal in certain parameter ranges, i.e. the LP bound equals the dual Plotkin bound for these parameters. We will extend this result for $q \geq 3$ by giving a sufficient condition for the optimality of the dual Plotkin bound.

Acknowledgements: Supported by the Austrian Research Foundation (FWF), Projects P18455 and S9609.

Numerical investigations of hyperplane nets. **Gottlieb Piršić** (RICAM Linz, Austria) IC/MT1419/0

Cyclic nets and hyperplane nets are a recently defined class of digital nets, introduced by Niederreiter and further investigated by Dick, Pillichshammer and Pirsic.

Their definition has some relations to coding theory and is conceptionally quite simple. Nevertheless, indicated by some theoretical results, they seem to range through a fairly large subspace of all posssible digital nets.

In the talk some numerical investigations will be presented that shall aim at supporting this feeling. In particular, hyperplane nets constructed by the component-by-component method shall be considered, investigating the relations between the chosen weight structure and the t-parameter.

IC/MP96/022: Modern constructions of low-discrepancy sequences. #2

Organiser: Friedrich Pillichshammer (Universität Linz, Austria)
Co-organiser: Peter Kritzer (Universität Salzburg, Austria)

(For abstract, see session #1 above.)

A new quadrature using integration lattices. **Rong-Xian Yue** (Shanghai Normal University, PR China) IC/MT1509/0

In this paper we propose a new quadrature rule via approximating Fourier coefficients of variable transformed integrand with multidimensional integration lattice. The error analysis is derived for the proposed rule. A comparison is done between the new rule and the periodizing transformation methods. It is shown that the new rule improves the periodizing transformation methods.

This is a join work with Professor Fred J. Hickernell and Xiaoyan Zeng (Department of Applied Mathematics, Illinois Institute of Technology, Chicago, USA).

On component-by-component constructions. **Dirk Nuyens** (Katholieke Universiteit Leuven, Belgium), Ronald Cools (Katholieke Universiteit Leuven, Belgium) IC/MT1738/0

Since the initial work by Sloan and his collaborators on the component-by-component construction of good lattice rules, a lot of variations on this theme have been published. These include various function spaces, prime and composite number of points, intermediate-rank rules, polynomial lattice rules and extensible rules. In this talk we look at all these different constructions and how they connect to the fast component-by-component construction variant.

Construction of low-discrepancy point sets of small size. **Michael Gnewuch** (Universität Kiel, Germany) IC/MT1598/0

The worst-case error of high-dimensional numerical integration of certain function classes is intimately related to the star-discrepancy via inequalities of Koksma-Hlawka type. The essence here is that sample points with small discrepancy lead to small integration errors.

There are many constructions of n-point sets in the d-dimensional unit cube $[0,1]^d$ known whose star discrepancy is bounded from above by $O(n^{-1}\ln(n)^{d-1})$. This upper bound is believed to be asymptotically optimal. However, it is only helpful for n exponentially large in d, since $n \mapsto n^{-1}\ln(n)^{d-1}$ is an increasing function for $n \le e^{d-1}$. Additionally, for many constructions the implicit constants in the O-notation depend critically on d.

In high-dimensional numerical integration one cannot afford to use a number of sample points exponentially in d. Furthermore, large constants are undesired. Therefore it is of interest to find useful upper bounds for the smallest possible star- discrepancy of moderate sample sizes, and to construct small samples satisfying these bounds. Heinrich, Novak, Wasilkowski and Woźniakowski (2001) proved the bounds

$$d_\infty^*(n,d) \le Cd^{1/2}n^{-1/2} \quad \text{and} \quad n_\infty^*(\varepsilon,d) \le C^2 d\varepsilon^{-2},$$

where $d_\infty^*(n,d)$ is the smallest possible star-discrepancy achieved by n points and $n_\infty^*(\varepsilon,d)$ is the cardinality of the smallest sample guaranteeing a star-discrepancy less or equal to ε. In the second bound the dependence on d is optimal. A drawback here is that so far no reasonable estimate for the universal constant C has been published. Furthermore, the proof of the bounds is probabilistic and not constructive. In the same paper the authors used a probabilistic argument based on Hoeffding's inequality that leads to asymptotically slightly weaker bounds with explicit small constants. By using reasonably good δ-covers these estimates have been improved by Doerr, Gnewuch and Srivastav (2005) to

$$d_\infty^*(n,d) \le kd^{1/2}n^{-1/2}\ln(n)^{1/2} \quad \text{and} \quad n_\infty^*(\varepsilon,d) \le k^2 d\varepsilon^{-2}\ln(\varepsilon^{-1}),$$

with a small konstant k (essentially we have $k=\sqrt{2}$). The probabilistic approach here has the advantage that it can be derandomized to construct small samples satisfying these bounds. This has been done by Doerr, Gnewuch and Srivastav (2005). The algorithm given there is essentially a point-by-point construction using the method of conditional probabilities and pessimistic estimators.

Our new approach is based on special δ-covers and on recent results on generating randomized roundings with cardinality constraints by Doerr (2006). Compared with the algorithm from Doerr et al. the new algorithm is easier to implement and has a reasonably better running time.

This is joint work with Benjamin Doerr.

Koksma–Hlawka-type inequalities of fractional order. **Josef Dick** (UNSW Asia, Singapore) IC/MT2061/0

The Koksma-Hlawka inequality states that the error of numerical integration by a quasi-Monte Carlo rule is bounded above by the variation of the function times the star-discrepancy. Here we relax the smoothness assumptions required in the Koksma-Hlawka inequality. We introduce Banach spaces of functions whose fractional derivative of order $\alpha > 0$ is in L_p. We show that if α is an integer and $p = 2$ then one obtains the usual Sobolev space. Using these fractional Banach spaces we generalize the Koksma-Hlawka inequality to functions whose partial fractional derivatives are in L_p.

IC/MP242/023: Robust integral equation methods for high-frequency problems.

Organiser: Ivan Graham (University of Bath, UK)
Co-organiser: Stephen Langdon (University of Reading, UK)

In this minisymposum we showcase recent advances in the design, analysis and implementation of frequency-robust integral equation methods for acoustic and electromagnetic wave scattering problems. Traditional methods for these problems, based on (piecewise) polynomial approximations, suffer from lack of robustness, i.e. the number of degrees of freedom typically has to increase proportional to the frequency. Better methods, which in some sense take account of the asymptotic behaviour of the solution at high frequency, have been proposed and resulting challenges (arising both in the analysis of these new methods and in their extension to practical geometries) will be the subject of this minisymposium.

High-frequency scattering by curvilinear polygons. **Stephen Langdon** (University of Reading, UK), Mosiamisi Mokgolele (University of Reading, UK), Simon Chandler-Wilde (University of Reading, UK) IC/MT1767/023

For problems of acoustic scattering by sound soft convex polygons, it has recently been demonstrated by Chandler-Wilde and Langdon that by including plane wave basis functions supported on a graded mesh in the approximation space, with smaller elements closer to the corners of the polygon, convergence rates that depend only logarithmically on the frequency of the incident wave can be achieved. In this talk, we investigate the extension of these ideas to problems of scattering by curvilinear polygons.

An hp-BEM for high-frequency scattering by convex polygons. **Markus Melenk** (TU Wien, Austria), Stephen Langdon (University of Reading, UK) IC/MT1752/023

Time harmonic accoustic scattering by a convex polygon is considered. S. Chandler-Wilde and S. Langdon have recently proposed an integral equation based method for the high frequency scattering problem. Using a detailed regularity analysis of the solution, they were able to design an h-version trial space that has approximation properties that depend only logarithmically on the wave number. The key features are a) the ability to identify the leading order (in the wave number) behavior of the solution and b) a precise characterization of the solution behavior near the vertices of the polygon. Since the approximation order is fixed, the achievable convergence rate is algebraic. In this talk, we extend their work to the hp-version of the BEM. It is shown that the solution can be approximated at an exponential rate from the trial space; the problem size required to achieve a given accuracy grows only logarithmically with the wave number. In this talk, we also address the question of how to set up the stiffness matrix with work independent of the wave number.

Bounds on oscillatory integral operators from high frequency. **Marko Lindner** (University of Reading, UK), Stephen Langdon (University of Reading, UK) IC/MT1753/023

The development of efficient numerical methods for the solution of high frequency scattering problems is an area that has received an enormous amount of recent interest. Some new integral equation methods (e.g. the methods proposed by Bruno, Geuzaine, Monro, Reitich 2004; Dominguez, Graham, Smyshlyaew 2006; Chandler-Wilde, Langdon 2006) have led to a dramatic reduction in the number of degrees of freedom per wavelength required to achieve an accurate solution, compared with more standard schemes. However, one theoretical question that remains to be answered for many of these schemes is the question of how the integral operators (both continuous and discrete) behave as the wavenumber tends to infinity. Numerical results appear to indicate that in many cases the dependence of the operator norms on the wavenumber may not be too severe. In this talk we discuss the derivation of some bounds on the norms of highly oscillatory integral operators arising from scattering problems, and we place these results in the context of stability and convergence estimates for approximation methods.

High-order boundary integral methods for Maxwell's equations using microlocal discretization and fast multipole methods. **Eric Darrigrand** (Université de Rennes I, France), Ludovic Gatard (Université de Bordeaux, France), Katherine Mer-Nkonga (Commissariat à l'Energie atomique, France) IC/MT1571/023

This paper deals with an efficient method used to solve the integral equations of B. Després regarding the time-harmonic Maxwell's equations in unbounded exterior domain for high frequencies. Our work consists in improvements of the coupling of the Microlocal Discretization (MD) and the Fast Multipole Method (FMM) using a high-order finite-elements approximation and filtering the transfer functions of the FMM which involves privileged directions in that application. The integral formulation of B. Després offers the advantage of a linear system which is well conditioned, hermitian and positive definite. This enables us to use methods based on the conjugate gradient. The Microlocal Discretization introduced by T. Abboud, J.-C. Nédélec and B. Zhou consists in an approximation of the phase of the unknown such that the new unknown is strongly less oscillating. Such a consideration leads to a discretization with a coarser mesh for the interpolation of the unknown. However, the calculation involved in the resolution of the system still requires a fine approximation of the geometry. A first work consisted in considering a double mesh: the unknown was defined on a coarse mesh and the approximation of the geometry on a fine mesh, both of them made of plane triangles. The matrix of reduced size was evaluated using a multilevel FMM (MLFMM). Though the first numerical results were very encouraging, they were not accurate enough for some applications. One could expect such observation because of the error estimates investigated by T. Abboud et al. A use of high-order finite elements which required an adaptation of the MLFMM, overcame that lack of accuracy. Moreover, a filter of the transfer functions of the MLFMM reduced the cost of the most expensive step of the MLFMM. After a thorough study of the complexity, we optimized those improvements of the coupling MD and MLFMM to obtain an accurate method of calculation of the matrix with a quasi-linear complexity.

IC/MP242/023: Robust integral equation methods for high-frequency problems. #2

Organiser: Ivan Graham (University of Bath, UK)
Co-organiser: Stephen Langdon (University of Reading, UK)

(For abstract, see session #1 above.)

Robust boundary-integral methods for high-frequency acoustic scattering. **Ivan Graham** (University of Bath, UK) IC/MT2377/023

In this talk we discuss the numerical solution of the problem of acoustic plane wave scattering by a 2D convex smooth sound-soft object using hybrid numerical-asymptotic methods. In recent joint work with Victor Dominguez and Valery Smyshlyaev we developed Galerkin methods with oscillatory basis functions for this problem and proved that the resulting discretisations are essentially uniformly accurate independently of the wave number. A key component of the analysis is a proper description of the asymptiotic behaviour of the solution in a format suitable for numerical analysis. This requires some further development of the classical asymptotics results for this problem. In this talk we describe the required asymptotics results and how they feed in to the design of robust numerical methods. The talk of Victor Dominguez in this minisymposium will give more deatils of the robust numerical method, its error analysis and implementation.

This is joint work with Victor Dominguez and Valery Smyshlyaev.

An asymptotic derived boundary-element method for high-frequency scattering problems in 2D. **Víctor Domínguez** (Universidad Pública de Navarra, Spain), Valery Smyshlyaev (University of Bath, UK), Ivan Graham (University of Bath, UK) IC/MT2120/023

This work concerns itself with the numerical solution of the acoustic scattering of plane waves by smooth convex curves in the high-frequency regime.

The problem is solved by boundary element methods using a direct approach with the normal derivative of the total wave as the new unknown of the problem. The normal derivative is then determined by solving an integral equation on the boundary, the so-called Burton-Miller equation. A complete analysis of the integral equation is developed in the circle where a deep Fourier analysis of the operator is possible. We prove that the condition number of the integral equation increases as $\mathcal{O}(k^{1/3})$, k being the wavenumber, and that the corresponding operator is actually coercive for all k high enough. These results, which have been also observed numerically in 2D, can be straightforwardly extended to spherical obstacles in 3D. As consequence we derive the stability of any Galerkin scheme with the Cea constant growing as $\mathcal{O}(k^{1/3})$.

To devise a method which is robust as the wavenumber k gets large, we use the known asymptotic form of the solution to obtain particular expansions in various zones of the boundary. These expansions allow to write the solution of the integral equation as a product of explicit oscillatory functions and more slowly varying amplitudes in each zone. The discrete spaces used polynomial approximations of the slow amplitude, as therefore can be understood as a sort of p method. In the shadow part a zero approximation is proposed and analytically justified as a good choice when k gets into the high frequency regime.

Our method is almost robust, suffering only from a very weak deterioration as $k \to \infty$ so that a slight increase in the dimension of the discrete space, taking the degrees of freedom as $k^{1/9}$ is a typical behaviour, preserves the accuracy of the numerical solution. Finally, we note that although the matrix of the method is relatively small, each entry is defined by a dou-

ble integral process where the integrand is highly oscillatory. It makes the classical quadrature rules prohibitely expensive to use and therefore different approaches should be considered to compute the integrals. We show some new results on this topic.

An efficient algorithm for high-frequency obstacle scattering in 3D. **Mahadevan Ganesh** (Colorado School of Mines, USA) IC/MT1179/023

We consider a surface integral equation formulation to model high-frequency scattering by a class of three dimensional obstacles. In recent years, there is some good progress in the development, implementation, and analysis of algorithms for high frequency scattering by two dimensional obstacles. However, it is still an open problem to develop corresponding practical algorithms for three dimensional scattering problems. In this work, we propose an efficient approach to simulate high frequency scattered and far fields generated by three dimensional obstacles that can be globally described in spherical coordinates.

Analysis of high-frequency multiple-scattering problems in 3D: the scalar acoustic and the vector electromagnetic equations. **Fatih Ecevit** (Max-Planck-Institut Leipzig, Germany) IC/MT1177/023

Recently developed numerical schemes, based on a combination of asymtotic theory and integral equations, provide very efficient strategies for the solution of high-frequency scattering problems. These methods, however, are strongly dependent on the underlying geometry, and are *mostly* restricted to single-scattering configurations. In this talk, we present a convergence analysis of a multiple-scattering algorithm for a collection of convex obstacles. To begin with, we show that the solution of the multiple-scattering problem can be attained through consideration of an iterative (Neumann) series (that successively accounts for further geometrical wave reflections and) that can be rearranged into a sum over primitive periodic orbits; then we analyze the properties of these periodic orbits in the high-frequency regime. To this end, we begin with a rigorous derivation of asymptotic expansions for the *currents* (i.e. the normal derivative of the fields) on arbitrary orbits, and carrying out a novel analysis of these expansions, we derive *precise analytical formulas* (for the scalar acoustic and vector electromagnetic equations) for the rate of decay of multiple scattering iterates on periodic orbits (of arbitrary period). Finally, we show that the convergence of the multiple-scattering iterates can be significantly improved utilizing these analytical formulas.

IC/MP671/023: Spectral computations for integral operators.

Organiser: Paulo Vasconcelos (Universidade do Porto, Portugal)
Co-organiser: Filomena d'Almeida (Universidade do Porto, Portugal)

Several problems in science and engineering can be modelled by integral operators on function spaces with interest on spectral computations. In this minisymposium we will survey methods for spectral problems dealing with operators defined on infinite dimensional domain and with infinite range. We will see how to approximate those operators by projecting them on finite dimensional subspaces, thus yielding large dimensional matrix spectral problems.

The solution procedures with preconditioning techniques and Krylov or Jacobi–Davidson type subspace methods will also be focused, in order to enlighten this crucial phase and to point out the need for the use of efficient and reliable linear algebra building blocks.

Spectral computations: from operators to matrices. **Filomena d'Almeida** (Universidade do Porto, Portugal), Paulo Vasconcelos (Universidade do Porto, Portugal) IC/MT4510/023

In this presentation we will address the problem of finding spectral values and basis for the corresponding invariant subspaces for bounded operators on Banach spaces. We will make a bridge between the spectral problem for the continuous operator and the computation of the eigenvalues and invariant subspace basis of a matrix. This matrix approximate problem is obtained with a convergent sequence of finite rank continuous operators followed by a restriction of these operators to a finite dimensional subspace. Subsequent defect correction procedures to refine the approximate solutions will also be addressed.

Building and solving matrix eigenproblems. **Mario Ahues** (Université Saint-Etienne, France) IC/MT1511/023

When infinite dimensional spectral problems are approximated through finite rank operator problems or slight perturbations of them, a matrix eigenproblem must be built and solved to compute eigenvalues and corresponding maximal invariant subspaces and eigenspaces.
This contribution covers
- A general theoretical framework for matrix problems issued from finite rank discretizations and perturbed variants,
- The stop criterion of the widely used QR method for the numerical computation of eigenvalues,
- The use of Newton-like methods to refine coarse approximate bases of maximal invariant subspaces in some special cases,
- The possibilities of using the Newton method to compute a Schur form of a complex square matrix as an alternative to the QR algorithm.

Comparison of parallel eigensolvers for a discretized radiative transfer problem. **Osni Marques** (Lawrence Berkeley National Laboratory, USA), Paulo Vasconcelos (Universidade do Porto, Portugal) IC/MT2510/023

In this work we consider the numerical computation of eigenelements of integral operators associated to a radiative transfer problem. This problem models the emission of photons in stellar atmospheres, and is formulated in terms of a weakly singular Fredholm integral equation defined on a Banach space. Computational approaches using direct and iterative strategies available in open source packages are discussed.

Computational challenges and algorithms in electronic structure calculations. **Yousef Saad** (University of Minnesota, USA) IC/MT3627/023

Density Functional Theory (DFT) is a successful technique used to determine the electronic structure of matter which is based on a number of approximations. It converts the original n-particle problem into an effective one-electron system, resulting in a coupled one-electron Schrödinger equation and a Poisson's equation. This coupling, which is nonlinear, involves the charge density which can be computed from the wavefunctions for all occupied states. These wavefunctions in turn are eigenfunctions of a Hamiltonian which depends (nonlinearly) on the charge density. This gives rise to a non-linear eigenvalue problem which is solved iteratively. The challenge comes from the large number of eigenfunctions to be computed for realistic systems with, say, hundreds or thousands of particles. We will discuss a parallel implementation of a finite difference approach for this problem and report on some results. The emphasis will be on solving the large eigenvalue problem. We will also explore the fundamental underlying linear algebra which can be viewed as a problem of determining the diagonal of a projector associated with an invariant subspace. Methods that avoid completely the computation of eigenvectors will be briefly discussed. Finally, we will present algorithms in time-dependent density functional theory with an emphasis on showing some of the resulting big challenges in matrix computation.

IC/MP118/024: The numerical solution of differential equations: recent advances.

Organiser: Paul Muir (Saint Mary's University, Canada)
Co-organiser: Raymond Spiteri (University of Saskatchewan, Canada)

The last few decades have seen a dramatic rise in the use of computational modelling as the primary tool for studying problems in applied and industrial mathematics. It is often the case that the underlying mathematical model is based on a system of differential equations. Increasingly however these models are more naturally formulated as differential–algebraic equations, i.e., differential equations augmented with algebraic equations that must also be satisfied. Applications experts who wish to perform computer simulations with these models continually attempt to study ever more sophisticated models that persistently push the limit of what can be handled with traditional numerical algorithms. Thus there is an ongoing need for the development of new computational techniques for the efficient, accurate, and robust simulation of such models. This mini-symposium brings together researchers who will discuss recent leading-edge advances in the algorithms and software for the numerical solution of differential equations. Topics include the numerical solution of boundary value differential equations with delay and advance terms, error estimation schemes for ODEs and DAEs, aspects of software development for systems of differential–algebraic equations, and a new class of waveform relaxation algorithms for large systems of ODEs arising from discretizations of partial differential equations.

Global a-posteriori *error estimates for index-1 DAEs.* **Ewa Weinmüller** (TU Wien, Austria), Winfried Auzinger (TU Wien, Austria), Herbert Lehner (TU Wien, Austria) IC/MT2675/024

We apply polynomial collocation to approximate solutions to index-1 DAEs in the form

$$A(t)\big(D(t)\,x(t)\big)' + B(t)\,x(t) = g(t)\,, \quad \text{for } t \in [0,1]\,,$$

where $A(t) \in \mathbb{R}^{m\times n}$, $D(t) \in \mathbb{R}^{n\times m}$, $B(t) \in \mathbb{R}^{m\times m}$, $g(t), x(t) \in \mathbb{R}^m$, with $n \le m$. For the numerical solution of the above system, we apply polynomial collocation to the enlarged system:

$$A(t)\,u'(t) + B(t)\,x(t) = g(t)\,, \qquad D(t)\,x(t) - u(t) = 0\,, \quad \text{for } t \in [0,1]\,.$$

Here, we focus on DAEs with so-called *properly stated leading term*, and use a Defect Correction principle to derive a posteriori error estimates for the global discretization error of the collocation scheme. Our procedure generalizes similar techniques which have proved useful in the ODE setting. The main idea of the error estimation procedure is to compute an appropriate defect measuring the quality of the collocation solution, and to apply a low-effort auxiliary scheme (backward Euler) with the defect as an additional inhomogeneous term. This leads the construction of an asymptotically optimal error estimate. In this procedure, local quadrature means of the continuous, pointwise defect of the collocation polynomial are used. We demonstrate that this strategy results in an asymptotically correct error estimate provided the problem data are appropriately smooth, and we illustrate the performance of our strategy by numerical experiments.

Some software aspects of DAEs and optimization software. **Stephen Campbell** (North Carolina State University, USA) IC/MT3676/024

Direct transcription methods have been successfully used to solve a variety of optimal control problems for some time. They are used in a number of codes such as the SOCS software developed at Boeing. In recent years it has begun to be realized that the existing computational theory needs to be modified when talking about direct transcription methods and the solution of constrained optimal control problems where DAEs arise. In addtion some modifications of the existing approach may be necessary if the approach is going to be extended to an even wider class of problems in order to encompass more applications. In this talk we will present two illustrations from our current investigations. Two examples are: use of the theory for constrained differential equations and DAEs and their implications for advice to users, and estimation of adjoint variables.

Algorithms for advanced–retarded differential equation boundary value problems. **Antony Humphries** (McGill University, Canada) IC/MT3345/024

Advanced–Retarded Functional Differential Equations arise in a wide range of applications, recently receiving attention because travelling wave solutions to lattice differential equations are defined by FDE boundary value problems on an unbounded domain. For example, the spatially discrete Nagumo equation

$$\dot{u}_i = u_{i+1} - 2u_i + u_{i-1} - \beta u_i(u_i - a)(u_i - 1), \quad i \in \mathbb{Z}$$

admits travelling waves of the form $u_i(t) = \varphi(i - ct)$ where the waveform $\varphi : \mathbb{R} \to \mathbb{R}$ and wavespeed c satisfy

$$-c\varphi'(\xi) = \varphi(\xi+1) - 2\varphi(\xi) + \varphi(\xi-1) - \beta\varphi(\xi)(\varphi(\xi) - a)(\varphi(\xi) - 1),$$
$$\varphi(-\infty) = 0, \varphi(+\infty) = 1.$$

The presence of advances as well as delays complicates the analysis and numerics of these problems, with the corresponding IVP being ill-posed. Also, the phenomenon of propagation failure, where a standing rather than travelling wave is observed, is represented by a singular limit in the FDE. Two numerical approaches for solving such problems will be presented, firstly by directly solving the BVP using a suitable collocation method, and secondly by using a travelling coordinate embedding. The truncation of the problem to a finite computational domain including the definition of suitable suitable implicit boundary functions, and validation of the algorithms will be discussed. Travelling waves in the spatially discrete Nagumo equation illustrate the issues that arise.

Optimized Schwarz-waveform relaxation algorithms for advection-diffusion problems. **Martin Gander** (Université de Genève, Switzerland) IC/MT4273/024

Optimized Schwarz waveform relaxation algorithms are a new class of waveform relaxation algorithms for large systems of ordinary differential equations (ODEs) arising from discretizations of partial differential equations. Like for classical waveform relaxation algorithms, the system of ODEs is decoupled into subsystems, but then coupling conditions adapted to the physics of the underlying problem are used to re-couple the subsystems with an iterative process. For discretized advection diffusion problems, I will show how to determine the best coupling conditions in two classes of simple coupling conditions, and prove that the new algorithms are well posed and convergent, with a much better convergence rate than the one of the classical waveform relaxation algorithm. I will illustrate the analysis with numerical experiments.

IC/MP3861/024: Taylor-model methods and interval methods: applications.

Organiser: Markus Neher (Universität Karlsruhe (TH), Germany)

Interval arithmetic has been widely used in enclosure methods for almost 40 years. Today, it is a well established tool for the calculation of rigorous error bounds for many problems in numerical analysis. Interest in interval arithmetic has been primarily aroused by the limitations of the floating point number format used on digital computers. Interval arithmetic provides a tool for controlling roundoff errors automatically, by enclosing real numbers into intervals with machine representable bounds and performing interval arithmetic operations with directed outward rounding, such that the exact result of any arithmetic operation is automatically enclosed in a floating point interval, including roundoff errors. Interval analysis is also used for bounding all kinds of truncation errors: the truncation error of an infinite iteration, as in the interval version of Newton's method, the remainder term of a convergent series, discretization errors in the numerical solution of differential equations, etc.

Unfortunately, the utility of interval arithmetic is sometimes impaired by the dependency problem and the wrapping effect, which both can cause overestimation of the solution set of a given problem, such that the computed error bounds may become over-pessimistic in practical calculations. The dependency problem is the lack of interval arithmetic to identify different occurrences of the same variable. For example, $x - x = 0$ holds for each $x \in R$, but $X - X$ is evaluated as $\{x - y \mid x, y \in X\}$. This set includes nonzero numbers, if X is a real interval that contains two or more distinct numbers. The wrapping effect appears when overestimation is enforced by the enclosure of intermediate results into intervals.

To reduce overestimation, Taylor models have been developed as a symbiosis of a computer algebra method and interval arithmetic by M. Berz and his group since the 1990s. A Taylor model of a function f on some interval X consists of the Taylor polynomial p_n of order n of f and an interval remainder term I_n, which encloses the approximation error $|f - p_n|$ on X. In computations that involve f, the function is then replaced by $p_n + I_n$. The polynomial part is propagated by symbolic calculations, whereas the interval remainder term encloses all truncation and roundoff errors that appear in the computation. Software implementations of Taylor models have been applied to a variety of problems, such as global optimization problems, validated multidimensional integration, or the solution of ODEs and DAEs.

The minisymposium deals with the presentation and discussion of recent advances in Taylor model methods and interval methods for various applications.

Interval techniques for enclosures of regions of reachability and controllability and for guaranteed state and parameter estimation of dynamical systems. **Andreas Rauh** (Universität Ulm, Germany), Marco Kletting (Universität Ulm, Germany), Eberhard Hofer (Universität Ulm, Germany) IC/MT1968/024

In this presentation, interval techniques for calculation of outer and inner enclosures of regions of reachability and controllability of dynamical systems are presented. Both discrete-time and continuous-time systems are considered. The applied methods are capable of calculating state enclosures for systems with uncertain parameters, nonlinearities, and time-varying characteristics under the assumption of a predefined finite time horizon. Although both uncertain system parameters and bounded control variables are assumed to be represented by intervals, they have to be distinguished in reachability and controllability analysis. Both reachability and controllability of states must be proven for all possible parameter values but for at least one admissible control sequence. Typically, robustness specifications for controllers of dynamical systems are given in terms of bounds on the system's time response which must not be violated for any possible operating condition.

Robust control strategies for nonlinear systems usually rely on knowledge of all current states. However, the complete state vector is not always directly accessible for measurement. Then, observers are applicable to reconstruct state variables which are not measurable. Additionally, observers are used successfully to improve the measured information by recursive computation of estimates and fusion of information determined by different measurement devices. If guaranteed bounds of all uncertain parameters of a dynamical system (including sensor characteristics) and conservative bounds of all disturbances can be specified, the presented interval observer can provide guaranteed enclosures of all reachable states.

In combination with the above-mentioned techniques for calculation of interval enclosures of regions of controllability and reachability, a mathematical proof of admissibility and robustness of control strategies under consideration of the influence of state estimation techniques becomes possible.

Extensions of ValEncIA-IVP for reduction of over-estimation, for simulation of differential algebraic systems, and for dynamical optimization. **Andreas Rauh** (Universität Ulm, Germany), Ekaterina Auer (Universität Duisburg-Essen, Germany), Johanna Minisini (Universität Ulm, Germany), Eberhard Hofer (Universität Ulm, Germany) IC/MT1964/024

In this presentation, we first summarize the basic routines of the validated solver ValEncIA-IVP (VALidation of state ENClosures using Interval Arithmetic for Initial Value Problems, http://www.valencia-ivp.com/). ValEncIA-IVP computes interval enclosures of all reachable states of dynamical systems described by ordinary differential equations with both uncertain parameters and uncertain initial conditions. These enclosures consist of an arbitrary non-validated approximate solution and additive guaranteed error bounds which are determined by a fixed-point iteration.

Extensions which aim at the reduction of overestimation are necessary for the application of ValEncIA-IVP to high-dimensional real-world systems. Here, tight state enclosures for a sufficiently long time span are desired. However, the main drawback of most methods for overestimation reduction is an increase of the required computational effort. That is, an appropriate compromise between effort and simulation quality is necessary.

The first extension of ValEncIA-IVP is a consistency test eliminating subintervals of *a priori* enclosures computed by the basic version of this solver which originate from overestimation. The second is a new approach for tightening of the enclosures with the help of exponential terms, which prevents growth of the diameters of the computed state enclosures especially for simulation of asymptotically stable systems. Third, we demonstrate implicit integration techniques which can be applied in the consistency test for further reduction of overestimation.

Based on these algorithmic improvements, we develop a first approach to extend ValEncIA-IVP to the simulation of sets of differential algebraic equations. We conclude this presentation with an outlook on the integration of ValEncIA-IVP in an interval arithmetic algorithm for computation of optimal and robust control strategies for uncertain continuous-time processes.

Validated simulation of kinematics and dynamics of multibody systems using interval and Taylor-model-based methods. **Ekaterina Auer** (Universität Duisburg–Essen, Germany) IC/MT1153/024

During the last decades, computer assisted modeling and simulation of multibody systems gained in importance. Computers help to reduce the design and development time for new products and to substitute low cost "virtual" tests for expensive experiments on real life prototypes. Besides, various types of modeling software have found a market in industry owing to their ability to generate models from systems' descriptions automatically. However, the results are often unreliable due to either errors that are unavoidably generated by numerical solvers of differential (or algebraic) systems or inaccuracy induced by the idealization of the model itself. This fact forces developers of modeling software to look for more reliable options, one of which is the use of validated arithmetics and algorithms. The main reasons for choosing a validated approach are, first, the guaranteed correctness of results and, second, the ability to allow for uncertainty in parameters, which helps to provide more realistic models or take into account measurement errors.

In this talk, we would like to present an integrated environment for validated modeling and simulation of kinematics and dynamics of various classes of multibody systems SMARTMOBILE (**S**imulation and **M**odeling of dyn**A**mics in MOBILE: **R**eliable and **T**emplate-based) based on the non-validated tool MOBILE. We will discuss general approaches to validate the behavior of a mechanical system using an integrated environment, the design requirements for a validated modeling and simulation tool, the application of interval and Taylor model based methods to it, as well as our achievements and open problems. We will demonstrate the functionality of the new tool and the importance of application of validated techniques using a variety of toy and close-to-life examples.

An efficient distance algorithm for interval-based octrees with time–space coherence utilization. **Cornelius Grimm** (Universität Duisburg–Essen, Germany), Eva Dyllong (Universität Duisburg–Essen, Germany) IC/MT3924/024

Among other approaches, such as implicit surfaces, constructive solid geometry or boundary representations, octrees feature a powerful technique for the geometric modeling of an object. Three dimensional interval vectors are used to describe the nodes of the octree for a reliable and efficient realization of the hierarchical data structure.

In this paper, a new distance algorithm for rotated and translated octrees is presented. It is based on accurate algorithms that have been shown in [DyllLuth04,DyllLuth06], but involves interval arithmetic for reliable handling of rounding errors. Furthermore, time-space coherence is utilized to increase the efficency of sequential distance calculations: Additional 'color' information is attached to the octree nodes to speed up the distance calculation after a movement of the considered octrees.

IC/MP3861/024: Taylor-model methods and interval methods: applications. #2

Organiser: Martin Berz (Michigan State University, USA)
Co-organiser: Markus Neher (Universität Karlsruhe (TH), Germany)

(For abstract, see session #1 above.)

Verified high-order optimal control in space-flight dynamics. **Roberto Armellin** (Politecnico di Milano, Italy), Pierluigi Di Lizia (Politecnico di Milano, Italy), Martin Berz (Michigan State University, USA) IC/MT2954/024

Space trajectory design always requires the solution of an optimal control problem in order to maximize the payload launch-mass ratio while achieving the primary mission goals. A certain level of approximation always characterizes the dynamical models adopted to perform the design process. Furthermore the state identification is usually affected by navigation errors. Thus, after the nominal optimal solution has been computed, a control strategy that assures the satisfaction of mission goals in the real scenario must be implemented. Traditional methods consist in non-optimal strategies mainly based on tracking the optimal solution, whereas the effectiveness of the synthesized control law is assessed by expensive Monte Carlo simulations.

In this frame Differential Algebra techniques are proposed as an effective alternative tool to design the control law, whereas Taylor models are subsequently applied to gain a validated controlled solution. By using Differential Algebra the final state dependency on initial conditions, environmental and control parameters is represented by high order Taylor Series expansions. The mission constraints and optimality conditions can then be resolved to higher order using a so-called high order partial inversion of the polynomial relationship for every admissible uncertainty. The control strategy is eventually reduced to a simple function evaluation. The flow of the resulting controlled dynamics is then computed using the verified integrator COSY-VI and a validated enclosure of the solution is obtained. As a result no further analysis on the effect of the uncertainties is required and the use of Monte Carlo simulations is avoided.

The performances of the proposed methods have been assessed by several examples of space mission trajectory design including an Earth-Mars low-thrust interplanetary transfer, a continuous propelled lunar landing trajectory, and an aerocapture maneuver at Mars.

Rigorous global optimization of multiple gravity-assist space trajectories. **Pierluigi Di Lizia** (Politecnico di Milano, Italy), Roberto Armellin (Politecnico di Milano, Italy), Martin Berz (Michigan State University, USA) IC/MT3036/024

Fuel efficient transfer from Earth to outer planets is often performed by means of multiple gravity assists, i.e. the close passing in the vicinity of one or more intermediate planets. The gravitational pull of the moving bodies can be used to increase velocity of the spacecraft and suitably alter its direction. The resulting problem is a constrained global optimization problem, where launch and transfer times between each of the assist planets are the free variables, and constraints are imposed in terms of the Lambert problem due to the necessity to connect two subsequent planets by a Keplerian conic arc.

In the last two decades, space trajectory designers have exploited the benefits of approaching the complex multiple gravity assist interplanetary transfer problem from a global optimisation standpoint. Nowadays, the aim of the trajectory design is not only to find a solution, but also to find the best solution in terms of propellant consumption, while still achieving the mission goals. Unfortunately, the multiple gravity assist interplanetary transfer problem is characterized by an objective function having a large number of clustered minima prevalently due to the complex relative motion of the planets involved in the transfer. This causes local optimisation gradient-based methods to converge to one of this local minimum. Consequently global optimization algorithms should be used.

Taylor model-based global optimization techniques are applied to determine rigorous global optima of the orbits over certain ranges of launch times and arrival times. The problem is practically complicated due to the abundance of local minima, a noticeable dependency problem since times allocated for one planet-connecting arc will influence subsequent maneuvers, and the relatively high dimensionality of the problem.

The performances of the proposed methods are assessed by means of classical multiple gravity assist interplanetary transfer test problems.

Implementing Taylor-model arithmetic with floating-point arithmetic. **Nathalie Revol** (École Normale Supérieure de Lyon, France) IC/MT2423/024

The implementation of Taylor models arithmetic may use floating-point arithmetic to benefit from the speed of the floating-point implementation. The issue is then to take into account the roundoff errors and to add them to the interval remainder. This ensures that the containment property is preserved. Here, we assume that the floating-point arithmetic is compliant with the IEEE-754 standard.

We show how to get tight bounds of the roundoff errors. The first operations we consider are the addition of two Taylor models or the product of a Taylor model by a scalar. Getting exactly the roundoff error of one single addition or multiplication involves the use of the TwoSum and TwoMult algorithms by Dekker and Veltkamp. These errors can be added together to the interval remainder. Various accurate summation algorithms have been developed, such as the one proposed by Rump, Ogita and Oishi. When two Taylor models are multiplied, each coefficient of the product is obtained via a dot product, which can again be computed accurately. The roundoff error for this dot product is thus tight.

Using these accurate techniques, we propose algorithms for the arithmetic operations on Taylor models. We then suggest to use polynomials of best approximation for the elementary functions, at least for the first approximations of low degrees.

Automatic strategies to evaluate formulas on Taylor models and generate proofs in PVS. **Francisco Cháves** (École Normale Supérieure de Lyon, France), Nathalie Revol (École Normale Supérieure de Lyon, France), Marc Daumas (Université de Perpignan, France), César Muñoz (National Institute of Aerospace, USA) IC/MT1724/024

Interval arithmetic [Moore 1966, Neumaier 1990, Jaulin *et al.* 2001] has been used in the last decades with successful results in science, mathematics and engineering. However, dependencies during the evaluation of formulas lead to overestimations of the returned results. Taylor Models have emerged as a convenient way to reduce this effect [Makino and Berz 2003]. They have also been used to solve initial value problems for ordinary differential equations as they provide a native guaranteed integration operator.

Interval Arithmetic as well as Taylor Models may be used to produce proofs as they yield enclosures of mathematical results. As more and more software is used to control devices that should never fail (for example software used for public transportation, medical care or weapons...), certification is now integrated with automated development tools such as the B toolkit or proof checking environment such as PVS [Owre *et al.* 1992].

We continued the development of our library of Taylor Models in PVS [Cháves and Daumas 2006] and we implemented the arctangent as needed to validate its polynomial approximation for example in KB3D or CRLIBM. We decided to work on the arctangent as it is clearly a full fledged example [Lester 2004] for the implementation of a new analytical operator to Taylor Model data type. Working with an automatic proof checker leads to the formalization of Taylor Models, i.e., the creation of a new data type and its operations along with proofs of correctness. Our library relies on PVS interval arithmetic library and strategies [Daumas, Melquiond and Muñoz 2005].

To offer *invisible formal methods* to users [Tiwari *et al.* 2003] we provide new strategies to recursively apply operators on Taylor Models, with as few intervention of the user as possible. With these strategies, users can quickly evaluate a formula and translate it into a fully qualified proof certified by PVS.

IC/MP95/024: Taylor-model methods and interval methods: techniques.

Organiser: Kyoko Makino (Michigan State University, USA)
Co-organiser: Markus Neher (Universität Karlsruhe (TH), Germany)

Interval arithmetic has been widely used in enclosure methods for almost 40 years. Today, it is a well established tool for the calculation of rigorous error bounds for many problems in numerical analysis. Interest in interval arithmetic has been primarily aroused by the limitations of the floating point number format used on digital computers. Interval arithmetic provides a tool for controlling roundoff errors automatically, by enclosing real numbers into intervals with machine representable bounds and performing interval arithmetic operations with directed outward rounding, such that the exact result of any arithmetic operation is automatically enclosed in a floating point interval, including roundoff errors. Interval analysis is also used for bounding all kinds of truncation errors: the truncation error of an infinite iteration, as in the interval version of Newton's method, the remainder term of a convergent series, discretization errors in the numerical solution of differential equations, etc.

Unfortunately, the utility of interval arithmetic is sometimes impaired by the dependency problem and the wrapping effect, which both can cause overestimation of the solution set of a given problem, such that the computed error bounds may become over-pessimistic in practical calculations. The dependency problem is the lack of interval arithmetic to identify different occurrences of the same variable. For example, $x - x = 0$ holds for each real number x, but $X - X$ is evaluated as $\{x - y \mid x, y \in X\}$. This set includes nonzero numbers, if X is a real interval that contains two or more distinct numbers.

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The minisymposium deals with the presentation and discussion of recent advances in Taylor model methods and interval methods for various applications.

Introduction to Taylor-model methods. **Markus Neher** (Universität Karlsruhe (TH), Germany) IC/MT1714/024

Interval arithmetic is used in enclosure methods for the calculation of rigorous error bounds for many problems in numerical analysis, such as truncation errors of infinite iterations or discretization errors in the numerical solution of differential equations. Interval arithmetic also provides a tool for controlling roundoff errors in computations with floating point numbers on digital computers automatically, by enclosing real numbers into intervals with machine representable bounds and performing interval arithmetic operations with directed outward rounding, so that the exact result of any arithmetic operation is automatically enclosed in a floating point interval, including roundoff errors.

Unfortunately, the utility of interval arithmetic is sometimes impaired by the dependency problem and the wrapping effect, which both can cause overestimation of the solution set of a given problem, such that the computed error bounds may become over-pessimistic in practical calculations. To reduce overestimation, Taylor models have been developed as a symbiosis of a computer algebra method and interval arithmetic by M. Berz and his group since the 1990s. A Taylor model of a function f on some interval X consists of the Taylor polynomial p_n of order n of f and an interval remainder term I_n, which encloses the approximation error $|f-p_n|$ on X. In computations that involve f, the function is then replaced by $p_n + I_n$. The polynomial part is propagated by symbolic calculations, whereas the interval remainder term encloses all truncation and roundoff errors that appear in the computation. Software implementations of Taylor models have been applied to a variety of problems, such as global optimization problems, validated multidimensional integration, or the solution of ODEs and DAEs.

Our presentation opens a minisymposium on interval methods and Taylor model methods. After an introduction to the basic concepts, we review interval methods and Taylor model methods for various applications.

Efficient Taylor-model-based verified ODE and flow integration using differential-algebraic methods. **Martin Berz** (Michigan State University, USA), Kyoko Makino (Michigan State University, USA) IC/MT3148/024

First we review various methods to provide verified enclosures of the flow of ODEs with a particular emphasis on efficiency. Then we analyze a new method based on establishing the defect of an approximation of the flow by its Taylor polynomial of order n in time and order k in initial conditions, and verified integration of this defect using Taylor model methods.

As is commonly done, first the Taylor time expansion of the center point of the domain of interest is determined as in conventional Taylor integrators. In the second step, the ODE is transformed to relative coordinates around the thus obtained center solution. By using Taylor model arithmetic, a representation of the ODE in these relative coordinates is obtained directly to high order.

In the third step, the Taylor representation of the flow of this ODE is obtained from the Taylor representation of the ODE in relative coordinates using differential algebraic methods, in particular a truncation of the exponential series of the Lie derivative of the flow. Again this step is directly possible using Taylor model arithmetic. For efficiency, it is most important that this step does not require any additional evaluations of the right hand side.

In the final step, an additional transformation to relative coordinates is performed, this time around the flow obtained in the third step. The resulting ODE, when evaluated in Taylor model arithmetic, consists of a vanishing polynomial part and a very small remainder bound. This resulting ODE can be trivially verified by a slope argument.

A comparison with the conventional TM-based verified integration algorithm is performed, showing the merits of the new approach for various problems. Some applications of the method will be presented.

Taylor-model-based enclosure of invariant manifolds for planar diffeomorphisms and applications. **Johannes Grote** (Michigan State University, USA), Martin Berz (Michigan State University, USA), Kyoko Makino (Michigan State University, USA) IC/MT3157/024

Fundamental questions in the study of interesting dynamics of planar diffeomorphisms like the Henon map involve homoclinic phenomena, topological entropy and strange attractors. Inherently, answering these questions requires knowledge about the stable and unstable manifolds, which in the typical case in the plane are smooth curves. We present a method that combines Taylor Model arithmetic with normal-form-transformation based techniques to find highly accurate Taylor Model enclosures of the invariant curves near hyperbolic fixed points. Successive iteration of these local manifold enclosures yields similarly accurate enclosures of significant pieces of the global invariant manifolds. Applications presented include the automatic computation of rigorous accurate enclosures of all homoclinic points in the manifold tangle up to finite iterates. Examples for cases with several thousand homoclinic points are given. This enables us to find symbolic dynamics in the underlying system and consequently compute rigorous lower bounds for its topological entropy.

Analysis of the blunting anti-wrapping strategy. **Kenneth Jackson** (University of Toronto, Canada), Markus Neher (Universität Karlsruhe (TH), Germany), Ned Nedialkov (McMaster University, Canada) IC/MT2744/024

Berz and Makino proposed the *blunting method* for reducing the wrapping-effect in their Taylor-model method for the validated numerical solution of initial-value problems for ordinary differential equations. The blunting method can be viewed as a combination of the well-known parallelepiped and QR-factorization methods for reducing the wrapping effect. We analyze the blunting method and show that, over sufficiently long integration intervals, it behaves like the QR-factorization method.

IC/MP95/024: Taylor-model methods and interval methods: techniques. #2

Organiser: Kenneth Jackson (University of Toronto, Canada)
Co-organiser: Markus Neher (Universität Karlsruhe (TH), Germany)

(For abstract, see session #1 above.)

Reliable safety analysis with continuous-time models. **Mark Stadtherr** (University of Notre Dame, USA), Youdong Lin (University of Notre Dame, USA) IC/MT2026/024

Safe operation has always been a key goal in the design and control of modern technological systems. Quantitative, model-based tools for safety analysis are a relatively recent development and, because of the computational challenges involved, have often been restricted to situations that can be described by fairly simple models. A further challenge is dealing with model uncertainty, indicating possible discrepancies between the mathematical model and the physical system whose safety is being studied.

Generally, a system may be considered unsafe when, under influence of external disturbances or equipment failure, it can reach certain undesirable states. In other words, from a given set of possible initial conditions and inputs and a finite time horizon, the goal is to determine the parts of this set for which safe operation can be guaranteed at all times. This problem has been addressed for some simple discrete time models [1,2]. In this study, we will use more realistic continuous-time models with uncertain parameters to represent the processes under consideration. Uncertain parameters are treated as intervals instead of probability distributions since safety analysis is concerned with the possibility for hazards to occur rather than with their likelihood. A validating parametric ODE solver, VSPODE [3], employing interval and Taylor model methods, will be used to simulate and bound trajectories in the interval-valued dynamic model. In this way, we are able to devise an approach for identifying the regions of operation that are guaranteed to be safe. Examples are used to demonstrate the potential of this approach for reliable safety analysis.

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High-order box rejection and pruning for global optimization based on Taylor-model methods. **Kyoko Makino** (Michigan State University, USA), Martin Berz (Michigan State University, USA) IC/MT3161/024

We develop two independent methods that allow box rejection and pruning for rigorous global optimization. Both methods are applicable for the use with Taylor model methods, which allow high-order dependency reduced relaxations of the optimization problem at hand.

The first method is applicable to convex functional relaxations over convex domains, which is characteristic of the situation near isolated minimizers where box rejection and reduction is often most difficult. It is based on an order-by-order decomposition of a general multivariate polynomial with positive definite quadratic part into a polynomial that is known to be positive definite to order n, and a remainder term of order n+1. As such, box rejection and domain pruning can be performed with an accuracy of order n+1.

The other method is based on a simplified version of the Taylor model based high-order inversion method that allows derivative-based exclusion of boxes in a global optimization setting. The use of Taylor models and the high-order inversion allows to do so with a sharpness that scales with the n-th power of the width of the domain boxes. Various examples for the practical use of the method are given, showing both the behavior for specific test cases and in a verified global optimization setting.

The practical use of the method greatly benefits from a method that allows the efficient calculation of (n-1)st order Taylor models (TM) for the gradient of a function in v variables simultaneously with the calculation of the Taylor model of the original function. The method is based on the well-known fact that the derivative of a Taylor polynomial of a function f equals the Taylor polynomial of the derivative of f to one less order. Thus, the knowledge of the Taylor polynomial coefficients of f to order n allows the direct determination of those of its partials by simple manipulation of the coefficients. To obtain the Taylor models for the gradient, it is hence only necessary to also accumulate v additional remainder bounds for the partials. An arithmetic is introduced that achieves this in a seamless way in parallel to conventional TM arithmetic. In typical cases of dimensions 5 to 20, the increase in computation time compared to a regular TM evaluation of the function alone is less than a factor of two.

A highly-accurate high-order verified method to solve the 3D Poisson equation. **Shashikant Manikonda** (Argonne National Laboratory, USA), Martin Berz (Michigan State University, USA), Kyoko Makino (Michigan State University, USA) IC/MT3120/024

The 3D Laplace and Poisson equations are important PDEs of Physics, describing the phenomenology of electrostatics and magnetostatics. For many practical problems, very precise and verified solutions of this PDE are required; but with conventional finite element or finite difference codes this is difficult to achieve because of the need for an exceedingly fine mesh which leads to often prohibitive CPU time.

We present an alternative approach based on high-order quadrature and a high-order finite element method. Both of the ingredients become possible through the use of Taylor model methods. In this approach we decompose the problem of solving the Poisson equation into the problem of solving the Laplace equation and finding the magnetic field due to an arbitrary source distribution. The underlying theory to find verified solutions to both these problems using Taylor model methods is developed. We then present various examples to demonstrate the accuracy achieved using this approach.

Guaranteed affine bound-functions for smooth functions based on Bernstein and Taylor expansion. **Jürgen Garloff** (HTWG Konstanz, Germany), Andrew Smith (HTWG Konstanz, Germany) IC/MT3842/024

A method for the computation of tight affine lower bound functions for arbitrary sufficiently often differentiable functions is presented. These bound functions may be employed in branch and bound algorithms for constrained global optimization problems, or any other application where linear underestimators or relaxations are used. An affine lower bound function is a simple type of convex underestimator which provides more information than merely the use of bounds on the range of a function. If such functions are used to construct relaxations for a global optimization problem, then sub-problems over boxes can be reduced to linear programming problems, which are easier to solve.

Our approach relies on the use of Bernstein expansion and Taylor expansion. Firstly, a Taylor polynomial approximation for the function over a specified box is computed. An affine lower bound function for the Taylor polynomial is computed by exploiting its expansion into Bernstein polynomials, and the associated coefficients. Interval arithmetic is employed to ensure a rigorous lower bound function. Secondly, the remainder of the Taylor expansion is enclosed in an interval, by using established methods from interval analysis. If a sufficiently high degree Taylor expansion is used in the first stage, then this remainder will be small. Subtracting this interval from the lower bound function for the Taylor polynomial provides the lower bound function for the given function.

Some examples will be presented to illustrate the performance of the algorithm. By altering the degree of the Taylor expansion used, a balance between the tightness of the resulting affine bound function and the speed of computation may be achieved.

IC/MP226/025: Mathematical analysis and numerical simulation for Bose-Einstein condensation.

Organiser: Weizhu Bao (National University of Singapore)
Co-organiser: Hailiang Li (Capital Normal University, PR China)

The experimental realization of Bose-Einstein condensates (BEC) in magnetically trapped atomic gases at ultra-low temperature has spurred great excitement in the atomic physics community and renewed the interest in studying the macroscopic quantum behavior of the atoms. Theoretical predictions of the properties of BEC like the density profile, collective excitations and the formation of quantized vortices can now be compared with experimental data. This dramatic progress on the experimental front has stimulated a wave of activity on both the theoretical and the numerical front. In this minisymposium, the speakers will address recent advancements in the following directions: (a). Mathematical analysis on existence and uniqueness of ground states as well as their asymptotics, stability and dynamical laws; (b). Efficient and accurate numerical methods for computing ground states and dynamics of BEC; (c). Dynamics of quantized vortices in BEC; and (d) Analysis and computation for quantum Boltzmann equation for BEC at finite temperature.

Quantized vortices in BEC and superconductors. **Qiang Du** (Pennsylvania State University, USA) IC/MT4147/025

Quantized vortices is a well-know signature of superfluidity. They have been studied extensively in superfluid Helium, type-II superconductors, Bose Einstein condensates and more recently in Fermi gas. We will discuss some mathematical analysis and numerical simulations of the quantized vortex nucleations in superconductors and Bose-Einstein condensates and discuss their connections and similarities.

Solitary waves in Bose-Einstein condensates with inhomogeneous nonlinearities. **Víctor Pérez-García** (Universidad de Castilla-La Mancha, Spain) IC/MT673/025

In this talk I will present several results on the existence, stability and dynamics of solitons in systems with inhomogeneous nonlinearities like Bose-Einstein condensates with spatially dependent scattering length. I will also present families of exact solutions and discuss several effects relevant for applications which can be obtained from the general theory.

Work done in collaboration with: Vadym Vekslerchik (U. Castilla-La Mancha), Juan Belmonte (U. de Castilla-La Mancha), H. Michinel (U. de Vigo) and P. Torres (U. de Granada)

Bifurcation analysis of Bose-Einstein condensates. **Shih-Feng Shieh** (National Taiwan Normal University) IC/MT1380/025

In this talk, we first prove that the solution curve of ground/positive bound states of a two component Bose-Einstein condensate(BEC)undergoes supercritical pitchfork bifurcations at some finite values of the inter-component scattering length. The ground state solutions bifurcate into two symmetric solutions with respect to some suitable axis on the symmetric domain, when a two-component BEC has equal intra-and inter-component scattering lengths. Second, we propose a Gauss-Seidel-type iteration(GSI)for the computation of energy states of a multi-component BEC. We prove that the GSI method converges locally and linearly to a solution of a nonlinear algebraic eigenvalue problem if and only if the associated minimized energy functional problem has a strictly local minimum. Numerical experience shows that the GSI converges globally within 10 to 20 steps.

A Hermite pseudo-spectral method for solving systems of Gross-Pitaevskii equations. **Rada Maria Weishäupl** (Universität Wien, Austria) IC/MT677/025

We propose and analyze discretization methods for solving finite systems of nonlinearly coupled Schrödinger equations, which arise as asymptotic limit of the three-dimensional Gross-Pitaevskii equation with strongly anisotropic potential. A pseudo-spectral method with Hermite basis functions combined with a Crank-Nicolson type method is introduced. Numerical experiments are presented, including a comparison with an alternative discretization approach.

IC/MP226/025: Mathematical analysis and numerical simulation for Bose-Einstein condensation. #2

Organiser: Weizhu Bao (National University of Singapore)
Co-organiser: Hailiang Li (Capital Normal University, PR China)

(For abstract, see session #1 above.)

Dynamics of rotating Bose-Einstein condensates and their efficient and accurate numerical computation. **Weizhu Bao** (National University of Singapore) IC/MT531/025

In this talk, we study the dynamics of rotating Bose-Einstein condensates (BEC) based on the Gross-Pitaevskii equation (GPE) with an angular momentum rotation term and present an efficient and accurate algorithm for numerical simulations. We examine the conservation of the angular momentum expectation and the condensate width and analyze the dynamics of a stationary state with a shift in its center. By formulating the equation in either 2D polar coordinate system or 3D cylindrical coordinate system, the angular momentum rotation term becomes a term with constant coefficients. This allows us

to develop an efficient time-splitting method which is time reversible, unconditionally stable, efficient and accurate for the problem. Moreover, it conserves the position density. We also apply the numerical method to study issues such as the stability of central vortex states and the quantized vortex lattice dynamics in rotating BEC.

This is a joint work with Qiang Du and Yanzhi Zhang.

Time-averaging and mathematical modeling of strongly confined Bose–Einstein condensates. **Florian Méhats** (Université de Rennes 1, France) IC/MT2123/025

This talk deals with a work in collaboration with F. Castella (Univ. Rennes, France) and N. Ben Abdallah (Univ. Toulouse, France).We study the limiting behavior of a nonlinear Schrödinger equation describing a 3 dimensional gas that is strongly confined along one or several directions. The confinement induces fast oscillations in time, that need to be averaged out. We analyze rigourously the convergence of a singularly perturbed equation towards a limiting model involving no oscillation. A key mathematical tool for this analysis is the use of almost periodicity.

Complex continuation for rotating Bose–Einstein condensates. **Cheng-Sheng Chien** (National Chung Hsing University, Taiwan) IC/MT1808/025

We study numerical solutions and trapping potentials of rotating Bose-Einstein condensates from the viewpoint of bifurcations. We show that the rotating BEC in the complex plane is governed by special two-coupled nonlinear Schrödinger equations (NLS) in the real domain. The locations of bifurcations are invariant under the affect of angular momentum. The wave functions of a rotating BEC can be easily obtained whenever the solution manifolds of the two-coupled NLS. We also study the bifurcation behavior when the 3D NLS is reduced to a 2D NLS. Numerical results on both the cylindrical domain and the 2D geometries reported. In particular, the numerical results show how the solutions of a single NLS are affected when an angular momentum is imposed on the equation. Moreover, the existence of the numerical solutions of the BEC depends on the choices of trapping potentials.

Numerical method for computing spin-1 Bose-Einstein condensate ground state. **Fong Yin Lim** (National University of Singapore), Weizhu Bao (National University of Singapore) IC/MT658/025

The imaginary time method and gradient flow with discrete normalization have been widely used to solve the Gross-Pitaevskii equation for single component BEC ground state. However, for spinor condensate with internal degree of freedom, difficulties arise as there are insufficient normalization conditions to normalize the coupled gradient flows at discrete time steps. In this presentation, a normalization condition is introduced for spin-1 condensate, in addition to the two existing conditions: the conservation of total particle numbers and the conservation of magnetization. The third normalization condition is derived from the relationships between the chemical potentials of each spinor components together with a splitting scheme applied to the coupled continuous normalized gradient flows. An efficient numerical method, the backward-forward sine-pseudospectral method (BFSP) that was developed to solve single component BEC ground state, is then extended to compute the ground state of spinor BEC.

IC/MP464/025: Efficient mass-conservative numerical schemes for multiphase and multicomponent flow and transport modelling environmental subsurface systems.

Organiser: Markus Bause (Universität Erlangen–Nürnberg, Germany)
Co-organiser: Florin Adrian Radu (Max-Planck-Institut Leipzig, Germany)

Reliable and efficient simulations of multiphase subsurface flows and contaminant transport phenomena are desirable in hydrological and environmental investigations, in civil and environmental engineering and for industrial oil exploration and production studies. The ability to model and simulate complex flows and reactive transport processes in composite soil formations is important from the point of view of physical realism. In this minisymposium recent developments and latest results in the application of numerical methods that are based on conservative techniques to the complex elliptic and parabolic model equations, also with degeneracy, describing such flows and transport phenomena are presented. In particular, mixed finite element methods including also higher order flux discretizations and finite volume based multipoint flux approximation schemes are considered. Various aspects of their analyses and practical implementation are addressed. The performance properties of the considered schemes are compared. The efficiency and reliability of these methods is illustrated by numerical convergence studies and for real-world subsurface flow and contaminant transport scenarios.

Properties of some locally-conservative numerical methods: application to reservoir simulation. **Runhild Klausen** (Universitetet i Oslo, Norway) IC/MT2107/025

The focus will be on discretization methods which are suited for the pressure equation as part of a multiphase subsurface flow problem. Extra focus will be given to various versions of the multi point flux approximations. Qualities, limitations and strengths of different versions of the methods will be discussed with respect to applications. Relationships to more classical methods like the mixed finite element methods will be shown and gains and losses discussed. In particular we will give a discussion on triangulations vs. quadrilaterals, robustness due to roughness in the grids and permeability, possibilities and effect of symmetry.

The work is done in collaboration with G.T. Eigestad, R. Winther and I. Aavatsmark.

Order of convergence estimates for a MFEM–Euler implicit scheme for a class of double degenerate parabolic equations. **Florin Adrian Radu** (Max-Planck-Institut Leipzig, Germany), Iuliu Sorin Pop (TU Eindhoven, The Netherlands), Peter Knabner (Universität Erlangen–Nürnberg, Germany) IC/MT1515/025

We consider here a class of nonlinear parabolic equations which can degenerate in the sense that the nonlinearity appearing in the time derivative can both vanish or blow up. As typical application we have in mind the Richards' equation, in its form after the Kirchhoff transformation, used for modeling saturated/unsaturated flow in porous media. We discretize in time by a scheme equivalent with Euler implicit and in space by the mixed finite element method (MFEM). Precisely, we use the lowest order Raviart-Thomas elements. Error estimates are presented to prove the convergence of the resulting fully discrete scheme. The advantage of the approach is that the convergence is obtained without any extra regularity assumptions.

The new results presented here extend the analysis done in [1].

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Higher-order mixed finite-element approximation of sub-surface water flow. **Markus Bause** (Universität Erlangen–Nürnberg, Germany) IC/MT1950/025

In this talk a higher-order finite element approach to variably saturated subsurface water flow and simultaneous (bio-)reactive multicomponent contaminant transport is considered. Higher order techniques have proved advantageous in the reliable and efficient simulation of biochemically reacting and mixing transport processes, due to their less amount of inherent numerical diffusion. Here, we focus in particular on a formally second-order accurate mixed finite element discretization of the parabolic-elliptic degenerate Richards equation, describing water flow in a variably saturated porous medium, by means of the lowest order Brezzi-Douglas-Marini element (BDM_1) and study the impact of the "improved" flux approximation on the transport processes. A new optimal order error estimate for the BDM_1 mixed discretization of a class of nonlinear problems and of the Richards equation is given. Moreover, the numerical performance properties of the BDM_1 approach are carefully compared to those of a first-order accurate Raviart-Thomas discretization (RT_0) and of a first-order accurate finite volume based multipoint flux approximation (MPFA). All these methods have in common that they are locally mass conservative. The comparison is done for various test cases. Finally, the application of the mixed finite element approach to subsurface water flow, with BDM_1 and RT_0 elements, is illustrated for some realistic complex field scale groundwater contamination scenarios with multicomponent reactive transport.

Entropy solutions of the Buckley–Leverett equation as limit of dynamic capillarity models. **Iuliu Sorin Pop** (TU Eindhoven, The Netherlands), van Duijn Hans (TU Eindhoven, The Netherlands), Peletier Bert (Universiteit Leiden, The Netherlands) IC/MT1565/025

We discuss an extension of the Buckley–Leverett (BL) equation describing two-phase flow in porous media. This extension includes a third order mixed derivatives term and models the dynamic effects in the pressure difference between the two phases. We derive existence conditions for traveling wave solutions of the extended model. This leads to admissible shocks for the original BL equation, which violate the Oleinik entropy condition and are therefore called nonclassical. In this way we obtain non-monotone weak solutions of the initial-boundary value problem for the BL equation consisting of constant states separated by shocks. Such results have been obtained experimentally. We conclude this talk by numerical experiments confirming the theoretical analysis.

IC/MP928/025: New directions in PDE simulations.

Organiser: David Bortz (University of Colorado at Boulder, USA)

Recent developments in numerical PDEs such as grid-free particle methods as well as fast-solver based boundary integral approaches suggest exciting possibilities for dramatic improvement in simulation time as well as physical realism. In some cases, the analysis of these methods do not easily lend themselves to traditional numerical analysis techniques. The purpose of this minisymposium is to showcase both the recent advances in PDE simulation approaches as well as novel approaches in studying the fidelity of the numerical simulation.

Numerical heating and particle codes. **Andrew Christlieb** (Michigan State Univsersity, USA) IC/MT3181/025

Plasmas (ionized gases) have rich and complex behavior which often need multiple lines of attack to fully understand their rich dynamics. Depending on the length scales involved, the plasma may be described by either a kinetic or a fluid model, the kinetic model being the more fundamental of the two. In this talk we will give a brief overview of the relation between these two models and then discuss Lagrangian particle methods for kinetic plasma problems. In particular, we will discuss the issue of numerical heating in a verity of grid-based and grid-free particle methods. This includes issue's of time stepping errors, mesh based effects, particle shape functions (type of regularization) and number of macro-particles. A further source of numerical heating is through the inclusion on inter-particle collisions via a monte-carlo approximation. It has been demonstrated that in 1D, the statistical error couples in a nonlinear way to the long range fields. We will spend the last portion of our talk discussing this issue.

Convergence analysis of grid-free PDE methods. **David Bortz** (University of Colorado at Boulder, USA), Andrew Christlieb (Michigan State Univsersity, USA) IC/MT3246/025

Grid-free numerical methods for solving PDE's have recently received considerable attention in the plasma simulation community. In this talk, we will present preliminary work on a novel framework for analyzing the convergence properties of this class of methods. The main idea of this framework focuses on employing statistical and connectivity properties of discretizations of differential operators to provide an alternative convergence metric.

Rapid evaluation of electrostatic interactions in multi-phase media. **Per-Gunnar Martinsson** (University of Colorado at Boulder, USA) IC/MT3370/025

In this talk, we will describe some fast numerical techniques for solving electro-statics problems involving a number of charged particles in a domain consisting of two or more regions with different dielectric constants. Such problems frequently need to be solved at each timestep in Monte Carlo or molecular dynamics simulations of biochemical phenomena, semi-conductors, etc. Since typically a very large number of problems need to be solved, computational speed is of crucial importance. For this reason, FFT-based solvers operating on equispaced grids have been a method of choice – in spite of a lack of rigorous error control, or the possibility of adaptive mesh refinement. In this talk, we will demonstrate that methods based on integral equation formulations can be as fast as, and sometimes substantially faster, than FFT-based methods. A principal advantage of integral equation based methods is that the discretization points are placed exactly at the locations where the physics is of interest (domain boundaries, charge locations, etc). This makes it possible to simultaneously achieve complete error control and superior computational speed.

Second-order embedded-boundary methods for electromagnetic particle-in-cell. **Matthew Bettencourt** (Air Force Research Lab., Kirtland AFB, USA) IC/MT3826/025

The mainstay of low density plasma simulations has been handled with electromagnetic particle-in-cell codes. These codes typically relied on the Finite-Difference Time-Domain algorithm for the electromagnetics and the Boris push with conservative current weighting by Villasenor and Buneman. These techniques suffer from a loss of accuracy near physical boundaries due to the stair-cased approximation. This talk outlines an approach to solving both the electromagnetics and the particle portions of this problem with cut-cell embedded boundaries, restoring second order accuracy and reducing the error by an order of magnitude.

IC/MP253/025: High-order shock capturing methods for non-linear hyperbolic partial differential equations.

Organiser: Miroslav Čada (ETH Zürich, Switzerland)
Co-organiser: Vincent Wheatley (ETH Zürich, Switzerland)

In recent years, there have been major advances in the design of numerical algorithms for solving non-linear hyperbolic conservation laws. In order to deal with problems involving long time dependency, multiple wave interactions, and discontinuous waves such as shocks and contact discontinuities, a numerical algorithm has to be fast, accurate and, in terms of shocks, non-oscillatory. To resolve the fine-scale features of a solution, turbulence being one example, it is also desirable for the algorithm to be high order accurate and have low numerical dissipation away from discontinuities. This challenge has led to a wide spectrum of possible methods. In general we can characterize three different groups, namely finite volume or finite difference methods, finite element methods and hybrid methods. In order to achieve better spacial resolution, high-order polynomial reconstructions and more recently non-polynomial reconstructions using hyperbolae and logarithmic functions have been used. These are then implemented in the context of finite volume or finite element methods using smoothness indicators to detect the presence of discontinuous waves. Hybrid methods adopt this idea, but try to combine shock capturing methods with, for example, spectral methods or high-order central differences. A major difficulty is the construction of a sophisticated smoothness indicator that can distinguish between smooth but narrow extrema and sharp discontinuities. We hope to explore both the present capabilities and limitations of these methods, along with what advances may be close at hand.

Shock-capturing schemes: high accuracy versus total-variation boundedness. **Antonio Marquina** (Departamento Matematica Aplicada, Universidad de, Spain), Susana Serna (University of California, Los Angeles, USA) IC/MT3758/025

High-order accurate shock capturing schemes are designed to resolve complex shock dynamics with high accuracy in space and time avoiding spurious oscillations near discontinuities. The presence of moving discontinuities in the flow at different scales makes this issue a computational challenge. We review different approaches from Lax-Wendroff and Van Leer pioneering contributions, through Harten total variation diminishing schemes (TVD) and essentially non oscillatory (ENO) piecewise polynomial schemes, to the more recent weighted ENO schemes and piecewise hyperbolic and logarithmic schemes. We discuss the use of slope limiters to reduce the degeneration in accuracy near discontinuities. We present a set of numerical experiments showing advantages and disadvantages of the different approaches.

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High-order well-balanced central schems on staggered grids, with application to shallow-water equations. **Giovanni Russo** (Università degli Studi di Catania, Italy), Alexander Khe (Lavrentyev Institute of Hydrodynamics, Russian Federation) IC/MT3848/025

A new family of high resolution shock captiring finite volume schemes is proposed for the numerical solution of systems of balance laws. Space-time discretization is obtained by the Central Runge-Kutta approach [1], previously introduced for the cnstruction of high order central schemes for conservation laws. High order non oscillatory property is obtained by the use of WENO reconstruction in space, and Runge-Kutta in time. The well-balanced property is guaranteed by performing the reconstruction in the so called equilibrium variables, rather than in the conservative of characteristic variables. A suitable map betwenn conservative and equilibrium variables, which preserves conservation, is used. Applications to the shallow water equations are presented. The numerical results illustrate the high order accuracy, and well-balanced property of the scheme, for perturbation around arbitrary equilibria.

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Central finite-volume and HLLC-type methods for hyperbolic systems and ideal MHD. **Paul Arminjon Paul** (Université de Montréal, Canada) IC/MT3989/025

Central Finite Volume methods , based on the staggered Lax-Friedrichs and Nessyahu-Tadmor one-dimensional Difference schemes , avoid the resolution of the Riemann problems generated at the cell interfaces thanks to the use of two staggered Grids at alternate time steps . Widely used and tested in applications to transonic/supersonic compressible flows using either Cartesian or Unstructured Triangular/Tetrahedric grids, they provide second-order accurate , computationally efficient and (in conjunction with appropriate limiters) non-oscillatory solvers for nonlinear hyperbolic systems.

We have recently adapted these methods to problems in ideal Magnetohydrodynamics, where we constructed appropriate extensions of Evans and Hawley's Constrained Transport method to satisfy the $\mathrm{div}\, B = 0$ constraint , and showed their feasibil-

ity, accuracy and robustness: even when we do not apply our CTCS divergence treatment to the magnetic field , our results remained meaningful , albeit not as accurate as when we apply this divergence treatment . We are also considering some versions of the HLLC Riemann solver for these problems , and compare the two approaches .

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High-order ADER finite-volume schemes for diffusion–reaction equations. **Eleuterio Toro** (Università degli Studi di Torino, Italy) IC/MT4011/025

We construct very-high order finite volume schemes for solving non-linear diffusion-reaction parabolic equations, following the ADER approach, first developed for hyperbolic equations [1]. A key step in the construction of the schemes is an approximation to the solution of a high-order Riemann problem for parabolic equations of the diffusion-reaction type. We note that the obvious generalization of the classical first-order Godunov scheme for diffusion leads to an inconsistent scheme. This difficulty is resolved in a very natural way by considering high-order Riemann problems, or derivative Riemann problems, as for the hyperbolic case [2], [3]. These are Cauchy problems in which the initial conditions are, for example, high-order polynomials in space and the sought solution at the interface is a high-order polynomial in time. The schemes are non-linear, the high-order representation of the polynomial data comes from a modified conservative ENO approach; the modification puts restrictions of the lengths of the stencils, based on accuracy and stability considerations.

Schemes of up to 10th order in space and time are implemented and assessed, with particular attention to the convergence rates of the schemes.

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IC/MP840/025: High-order methods for wave propagation and flow problems in complex geometries.

Organiser: Michael Dumbser (Universität Stuttgart, Germany)
Co-organiser: Eleuterio Toro (Università degli Studi di Torino, Italy)
Co-organiser: Claus-Dieter Munz (Universität Stuttgart, Germany)

This Minisymposium is concerned with latest developments on high order accurate numerical methods for constructing linear and non-linear numerical schemes of high order of accuracy in space and time for solving partial differential equations in multiple space dimensions on unstructured grids. The considered schemes are always time-accurate to compute transient phenomena, however, by construction they may easily incorporate local-time stepping to increase computational efficiency. Problems of interest involve wave propagation problems as well as flow and transport phenomena. One lecture will be devoted to provide a brief review of the ADER approach and of the basic ingredients, such as the solution of the Derivative (or Generalized) Riemann problem. Other lectures will address the design of ADER Finite Volume (ADER-FV) and ADER Discontinuous Galerkin (ADER-DG) schemes on unstructured meshes in multiple space dimensions for complicated domains, including high-order non-linear WENO reconstruction procedures on triangular and tetrahedral meshes. The workshop will also include several applications of the numerical methods to typical wave propagation and fluid flow problems that require the use of numerical schemes of high order of accuracy, namely elastic wave propagation in heterogeneous anisotropic viscoelastic material as well as compressible gasdynamics.

Approaches for solving the derivative Riemann problem. **Eleuterio Toro** (Università degli Studi di Torino, Italy) IC/MT4442/025

The Derivative (or higher-order) Riemann problem for non-linear systems of hyperbolic balance laws is the Cauchy problem for the relevant system of equations in which the initial conditions are piece-wise smooth. The motivation of this work is the construction of high-order Godunov type methods for conservations laws, called ADER methods. We present various techniques for obtaining solutions to this problem along time axis, as a time power series expansion. One method, first put forward by Toro and Titarev (2002), is based on a power series expansion of the sought solution at the interface position x=0. The leading term is found by solving a classical Riemann problem (piece-wise constant data) for the state variables and the coefficients of the higher-order terms in the expansion result from solving classical Riemann problems for space derivatives, after using the Cauchy-Kowalewski procedure. Another method of solution due to Castro and Toro (2006) results from a re-interpretation of the higher order method of Harten, Engquist, Osher and Chakravarthy (1987). Here, power series expansions on either side of the initial discontinuity are first written. The Cauchy-Kowalewski procedure allows the use of the initial conditions and the differential equations to define left and right states at any time. There follows the solution of a non-linear classical Riemann problem to find the solution of the higher-order Riemann problem at the given time at x=0. These methods work well for hyperbolic equations with non-stiff source terms. We also discuss a recent alternative method due to Dumbser, Enaux and Toro (2007) where the Cauchy-Kowalewski procedure inside each control volume is replaced by a local space-time discontinuous Galerkin scheme. We emphasize that with this new approach one can still construct non-oscillatory numerical methods of arbitrary order of accuracy in space and time for nonlinear systems of balance laws with source terms that may even be very stiff.

A discontinuous Galerkin scheme based on a space-time expansion. **Claus-Dieter Munz** (Universität Stuttgart, Germany) IC/MT4437/025

The class of discontinuous Galerkin (DG) schemes is interesting for practical calculations of problems in complex geometries, because the approximate solutions usually show the theoretical order of accuracy even on distorted unstructured grids. Due to the fact that the approximate solution in the DG schemes may be discontinuous at grid cell interfaces, they allow the approximation of strong gradients on coarse grids. In this talk we propose a discontinuous Galerkin scheme which is based on a space-time Taylor expansion about the barycenter at the old time level. All time or mixed space-time derivatives

are replaced by pure space derivatives using the evolutionary differential equation several times which is called the Cauchy-Kovalevskaya procedure. The Taylor expansion gives the values for the Gaussian quadrature rules which are applied to the surface and volume space-time integrals in the variational formulation. We discuss the numerical approximation of the advective as well as the diffusive fluxes between the grid cells.

The proposed scheme is used in a way such that it is locally adapted to the behavior of the solution. This includes h-adaptivity, which is especially efficient due to the possibility to have nonconforming mesh nodes, and p-adaptivity allowing the degree of the local approximation space to vary from element to element. The space-time expansion discontinuous Galerkin scheme (STE-DG) scheme is also locally adapted with respect to the time approximation. We have no longer a global time step, but each grid cell may evolve in time with a local time step corresponding to the local stability restrictions. This technique highly increases performance for multi-scale problems where the local time steps strongly vary over the computational domain.

We show an example for a simulation in aeroacoustics in which the noise generating region as well as the propagation of acoustic waves into the far-field are simulated. Another example is the simulation of fluid flow based on the compressible Navier-Stokes equations. The flexibility and adaptivity of the scheme allows to vary the order of the approximation as well as the grid cell size corresponding to local behavior of the solution, while the local time stepping always guarantees efficiency of the simulation on the entire domain.

The co-authors of this paper are Gregor Gassner and Frieder Lörcher

ADER Runge–Kutta methods for conservation laws. **Giovanni Russo** (Università degli Studi di Catania, Italy) IC/MT4484/025

A new family of high resolution finite volume schemes for the numerical approximation of solutions of conservation laws is presented. The schemes are based on a combination of ADER schemes with Central Runge-Kutta time discretization. In original ADER schemes, at the edge of each computational cell the so-called Derivative Riemann problem for the state variable u is posed with the initial left and right states provided by a suitable high order non oscillatory reconstruction, such as WENO. The solution is then given in a form of the Taylor expansion in time whose oefficients are expressed in terms of high order space derivatives, by successive differentiation of the governing equation.

In the new approach, the Taylor expansion in time is replaced by a Runge-Kutta scheme. Using the CRK approach, the conservative numerical solution for the cell average is expressed in terms of the stage values computed at theedge of the cell. The latter in turn are evaluated by a triangular approach: a p-stage scheme requires p-1 values of the space first derivative, computed by the evolution equation for u_x; such values require p-2 values of the second space derivative, and so on.

The overal procedure will provide essentially the same results of the original ADER scheme, but at a lower copmutational cost. Numerical results on one and two space dimensions will be presented.

Quadrature-free WENO finite-volume schemes for nonlinear hyperbolic systems on unstructured triangular and tetrahedral meshes in 2D and 3D. **Michael Dumbser** (Universität Stuttgart, Germany) IC/MT4430/025

In our talk we present a quadrature-free weighted essentially non-oscillatory (WENO) finite volume scheme of arbitrary high order of accuracy both in space and time for solving time-dependent nonlinear hyperbolic systems on unstructured triangular and tetrahedral meshes in two and three space dimensions, respectively. For high order spatial discretization, a WENO reconstruction technique provides the reconstruction polynomials in terms of a hierarchical orthogonal polynomial basis over a reference element. To ensure non-oscillatory behaviour also for nonlinear systems, characteristic reconstruction is used. The Cauchy-Kovalewski procedure applied to the reconstructed data yields for each element a space-time Taylor series for the evolution of the state and the physical fluxes. This Taylor series is then inserted into a new numerical flux which is a function of four arguments, namely the states and the physical fluxes on both sides of the interface, and which can then be subsequently integrated analytically in space and time. Thus, the Cauchy-Kovalewski procedure provides a natural, direct and cost-efficient way to obtain a quadrature-free formulation, avoiding the expensive numerical quadrature arising usually for high order finite volume schemes in three space dimensions. We show numerical convergence results up to sixth order of accuracy in space and time for the compressible Euler equations of gas dynamics on triangular and tetrahedral meshes in two and three space dimensions. Furthermore, various unsteady two- and three-dimensional flow problems with smooth and discontinuous solutions are computed to validate the accuracy of the approach and to underline the non-oscillatory shock-capturing properties of the method. To our knowledge, this is the first high order accurate quadrature-free WENO finite volume scheme ever presented for nonlinear hyperbolic systems on unstructured three-dimensional tetrahedral meshes. As a final outlook to future applications, first results for the compressible unsteady Navier-Stokes equations on unstructured triangular and tetrahedral meshes in two and three space dimensions are shown.

IC/MP32/025: Artificial boundary conditions for linear and nonlinear Schrödinger equations.

Organiser: Matthias Ehrhardt (TU Berlin, Germany)
Co-organiser: Xavier Antoine (Université Henri Poincaré Nancy I, France)
Co-organiser: Christophe Besse (Université Lille 1, France)

We discuss recent developments related to the numerical solution of time-dependent linear and nonlinear Schrödinger equations on unbounded domains. The eight speakers will focus on the three following topics which are of primary interest concerning Schrödinger-type equations:

1) recent approaches to implement the classical *transparent boundary condition* into finite difference and finite element discretizations for the one-dimensional problems;
2) new strategies to derive fast and stable implementations of the convolution operators involved in the definition of the *artificial boundary conditions* (ABCs); and
3) recent construction of ABCs for nonlinear (cubic) Schrödinger equations or/and for general geometries of the computational domain.

When computing numerically the solution of a linear or nonlinear partial differential equation in an unbounded domain, a fictitious boundary is usually introduced to limit the computational domain. Special boundary conditions are derived at this boundary to approximate the exact whole-space solution. If the solution of the problem on the bounded domain is equal to the whole-space solution (restricted to the computational domain) these boundary conditions are called exact or transparent boundary conditions (TBCs), otherwise they are called artificial boundary conditions (ABCs). Different strategies can therefore be developed. In this minisymposium we are planning to invite people who made recent developments on this subject for linear and nonlinear Schrödinger equations; e.g., the cubic Schrödinger equation. An example for a cu-

bic Schrödinger equation arises in nonlinear optics for laser beam propagation where the polarization of the material has a cubic nonlinearity due to the electric field. More applications stem from fiber optics communications, quantum mechanics or plasma physics.

In the case of a linear equation (even in the one-dimensional case), different complex questions must be considered

- How to derive a stable and accurate scheme for approximating the nonlocal convolution operator defining the boundary condition?
- How to build some accurate TBCs or ABCs for two-dimensional problems?
- Since the TBCs and ABCs include a convolution operator in time (and eventually space), with a weakly decaying kernel, its evaluation becomes very costly for long-time simulations. How to derive then some efficient evaluation algorithms for such operators to reduce the complexity?

These questions will be discussed in the first part of the minisymposium and the first talk of the second part.

While TBCs/ABCs for linear equations can be constructed via integral transformations (Laplace-, Fourier-, Z-transformation) the construction of continuous TBCs/ABCs for nonlinear Schrödinger equations is based on pseudo-differential and para-differential techniques and is far from being trivial. This area represents a current and challenging research topic which will be discussed during the second part of this minisymposium.

Construction of 2D artificial boundary conditions for the linear Schrödinger equation via fractional pseudo-differential operators. **Christophe Besse** (Université Lille 1, France), Xavier Antoine (Université Henri Poincaré Nancy I, France) IC/MT1529/002

A transparent boundary condition for the two-dimensional linear Schrödinger equation is constructed through a microlocal approximation of the operator associating the Dirichlet data to the Neumann one in a "M-quasi hyperbolic" region. To be usable, this condition must be approximated in a high-frequency regime by an asymptotic artificial boundary conditions which involves fractional derivatives with respect to the time variable. In such a way, these conditions present the features of being differential in space and non-local in time. Then, we address the construction and study of a Crank-Nicolson-type discretization of the two-dimensional linear Schrödinger equation in a bounded domain Ω with these artificial boundary conditions set on the arbitrarily shaped boundary of Ω. After having proved the well-posedness of the continuous truncated initial boundary value problem, a semi-discrete Crank-Nicolson-type scheme for the bounded problem is introduced and its stability is provided. Next, the full discretization is realized by the way of a standard finite-element method to preserve the stability of the scheme. Some numerical simulations are given to illustrate the effectiveness and flexibility of the developed method.

Exact absorbing boundary conditions for the Schrödinger equation with periodic potentials at infinity. **Chunxiong Zheng** (Tsinghua University, PR China) IC/MT5006/002

In this talk we will present a novel exact absorbing boundary condition for the Schrödinger equation with inversion-symmetric potentials at infinity. This boundary condition, in a form of Dirichlet-to-Neumann mapping, is based on an analytical expression of the logarithmic derivative of the Floquet solution to the Schrödinger equation. We will explain how we derive this expression and discuss the possibility of its extension to the more general case.

Absorbing boundary conditions for one-dimensional nonlinear Schrödinger equations. **Jérémie Szeftel** (Princeton University, USA) IC/MT3382/002

We construct two families of absorbing boundary conditions for the nonlinear Schrödinger equation. The first one relies on the reinterpretation of the nonlinear equation as a linear one with a potential term and the second one relies on the linearization of the equation. We then present numerical experiments illustrating the efficiency of these methods.

Construction and numerical approximation of artificial boundary conditions for a nonlinear Schrödinger equation. **Stéphane Descombes** (Ecole Normale Superieure de Lyon, France), Christophe Besse (Université Lille 1, France), Xavier Antoine (Université Henri Poincaré Nancy I, France) IC/MT2370/002

In this talk we give a construction of nonlinear artificial boundary conditions for the one-dimensional nonlinear cubic Schrödinger equation. Basically, the derivation consists in formally replacing the nonlinearity by a potential and constructing different kinds of approximate artificial boundary conditions for the resulting problem using the techniques of pseudodifferential calculus. Next, the potential is formally replaced by the nonlinearity. Numerical examples illustrate the efficiency of the non-linear artificial boundary conditions.

IC/MP32/025: Artificial boundary conditions for linear and nonlinear Schrödinger equations. #2

Organiser: Matthias Ehrhardt (TU Berlin, Germany)
Co-organiser: Xavier Antoine (Université Henri Poincaré Nancy I, France)
Co-organiser: Christophe Besse (Université Lille 1, France)

(For abstract, see session #1 above.)

A review of transparent and artificial boundary-condition techniques for linear and nonlinear Schrödinger equations. **Matthias Ehrhardt** (TU Berlin, Germany), Xavier Antoine (Université Henri Poincaré Nancy I, France), Anton Arnold (TU Wien, Austria), Christophe Besse (Université Lille 1, France), Achim Schädle (Zuse-Institut Berlin, Germany) IC/MT1425/002

In this review we discuss different techniques to solve numerically the time-dependent Schrödinger equation on unbounded domains. We present and compare several approaches to implement the classical *transparent boundary condition* into finite difference and finite element discretizations. We present in detail the approaches of the authors and describe briefly alternative ideas pointing out the relations between these works. We conclude with several numerical examples from different application areas to compare the presented techniques. Here we mainly focus on the one-dimensional problem.

Construction of stable discretization schemes of the transparent boundary. **Xavier Antoine** (Université Henri Poincaré Nancy I, France) IC/MT455/002

This talk will be devoted to the construction of stable discretization schemes associated with the linear one-dimensional Schrödinger equation. We will describe both the strategy to achieve this goal and a few numerical experiments showing that the method is effective.

WKB-schemes and open boundary conditions for quantum devices. **Anton Arnold** (TU Wien, Austria) IC/MT1609/002

We shall discuss two numerical tools that are crucial for numerical simulations of quantum wave guides in terms of the Schrödinger equation:

Firstly, we consider the stationary Schrödinger equation $-\epsilon^2\psi_{xx} + a(x)\psi = 0$ in both the oscillatory and the evanescant regimes. In the highly oscillatory case we discuss finite difference methods that do *not* require to resolve the oscillations. This can be achieved by a transformation that separates the oscillations from a slowly varying "envelope". In the evanescant regime we use a FEM with WKB ansatz functions of exponential type. Convergence, stability, and efficience of the resulting method are presented.

In the second part of the talk we present inhomogeneous transparent boundary conditions for the time-dependent Schrödinger equation.

Construction of transparent boundary conditions by the pole-condition method. **Frank Schmidt** (Zuse-Institut Berlin, Germany), Achim Schädle (Zuse-Institut Berlin, Germany), Daniel Ruprecht (Zuse-Institut Berlin, Germany), Lin Zschiedrich (Zuse-Institut Berlin, Germany) IC/MT2684/002

We present a general framework to treat the wave equation, the drift-diffusion equation, the heat equation, and the Schrödinger equation

$$\begin{aligned}
\partial_{tt}u(t,x) &= \partial_{xx}u(t,x) - k^2(t,x)u(t,x) \quad \text{(wave)}\\
\partial_t u(t,x) &= \partial_{xx}u(t,x) + 2d\partial_x u(t,x) - k^2(t,x)u(t,x) \quad \text{(drift-diffusion)}\\
i\partial_t u(t,x) &= \partial_{xx}u(t,x) - k^2(t,x)u(t,x) \quad \text{(Schrödinger)}
\end{aligned}$$

for $x \in \mathbb{R}$ and $t \geq 0$ complemented with appropriate initial conditions. The treatment is based on the pole condition concept and yields a general approach to all these different equations. The concept is not restricted to 1D spatial problems but generalizes directly to higher dimensions.

The basic idea of the pole condition approach is to consider the Laplace transform in space of u in the exterior of a bounded computational domain at each point in time. The function u is an outgoing wave with respect to the computational domain, if all poles of the Laplace transform of u are contained in a proper defined half-plane of the complex plane for all times. For the construction of the algorithm we use an indirect form of the pole condition in time. We study the position of the poles in the complex plane in dependence of the frequency of the Fourier transformed (in time) function u and require that all poles are contained in a proper defined half-plane of the complex plane for all positive frequencies. The definition of the half-plane depends on the nature of the equation and can be computed directly. The algorithmic realization of the pole condition yields constraints which become ordinary differential equations (ODEs) in time and which have to be solved together with the partial differential equation of the interior domain. The number of these additional ODEs determines the accuracy of the approximation in the exterior domain. Numerical tests for all equations yield exponential fast and stable convergence.

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IC/MP107/025: Recent advances in front propagation modelling and applications.

Organiser: Maurizio Falcone (Universita' di Roma "La Sapienza", Italy)
Co-organiser: Regis Monneau (Ecole Nationale des Ponts et Chaussées, France)

The numerical computation of the evolution of fronts is one of the most challenging problem with a large number of applications. Let us mention for instance the evolutions of free surfaces of fluids, shape optimization, the detection of contours in image processing, crystal growth and dislocations dynamics. In the last few years, there was a lot of progress in the understanding of these problems which has produced new models as well as new approximation schemes. All the above problems correspond to nonlinear evolutive partial differential equations which can be degenerate. Since the solution can develop singularities and the topology of the interface can change in finite time there is a need for highly accurate numerical methods which are stable with respect to those degeneracies. From the mathematical point of view, the notion of *viscosity solution* plays a crucial role to define the interface after the onset of singularities. In order to compute sharp interfaces, several techniques have been developed: adaptive finite elements, high order finite differences and semi-Lagrangian methods.

This minisymposium will focus on the most recent modelling of fronts evolutions and on accurate approximation methods to compute the solution of significant applied problems.

Tracking propagation of self-intersecting fronts: an invariant manifold approach. **Alexander Vladimirsky** (Cornell University, USA) IC/MT3701/025

In many front propagation problems, the front's position at the time t is represented as a particular level set of a solution to the corresponding first-order non-linear PDE. Typically, this PDE does not have a globally smooth solution and a unique (single-valued) viscosity solution is sought to automatically remove emerging self-intersections of the front. However, a smooth multi-valued solution is needed instead whenever the behavior of characteristics is still relevant even after their intersection (e.g., in geometric optics, multiple-arrival seismic imaging, and tomography).

Multi-valued solutions are frequently computed using Lagrangian methods (e.g., ray tracing) – solving the (2n-dimensional system of) characteristic ODEs for a finite number of initial conditions determined by the boundary conditions of the original PDE. The disadvantage of this approach is a poor spatial resolution due to a non-uniform rate of separation for trajectories of the ODE system. A number of Eulerian methods were proposed to alleviate this problem by solving a corresponding Liouville system of n linear PDEs in a 2n-dimensional (x,p) phase space.

We propose an alternative approach, which restricts the computations to an n-dimensional mesh approximating a particular invariant manifold of the characteristic vector field. That manifold is locally modeled as a graph of the function satisfying a quasi-linear flow-invariance PDE, which is then efficiently solved by a space-marching method in Eulerian framework. We illustrate our approach by computing multi-valued solutions for several Hamilton-Jacobi PDEs and hyperbolic conservation laws. This research is conducted in collaboration with J. Guckenheimer and J.A. Sethian.

High-order semi-Lagrangian contouring with complex moving interfaces. **John Strain** (University of California, Berkeley, USA) IC/MT1365/025

Models of physical phenomena such as crystal growth or blood flow generally involve complex moving interfaces, with velocities determined by interfacial geometry and material physics. Numerical methods for such models tend to be customized. As a consequence, they must be redesigned whenever the model changes.

We present a general computational algorithm for evolving complex interfaces which treats the velocity as a black box, thus avoiding model-dependent issues. The interface is implicitly updated via an explicit second-order semi-Lagrangian advection formula which converts moving interfaces to a contouring problem. Spatial and temporal resolutions are decoupled, permitting grid-free adaptive refinement of the interface geometry. A modular implementation computes highly accurate solutions to geometric moving interface problems involving merging, anisotropy, faceting, curvature, dynamic topology and nonlocal interactions.

A large time-step technique for geometric equations. **Roberto Ferretti** (Universita' Roma Tre, Italy), Elisabetta Carlini (Università degli Studi di Roma "La Sapienza", Italy), Maurizio Falcone (Universita' di Roma "La Sapienza", Italy) IC/MT3369/025

We present a strategy for constructing large time-step (or semi-Lagrangian) schemes for geometric equations arising in front propagation models, like advection-driven, eikonal and curvature-driven propagation. The scheme stems from a suitable representation formula for the solution and allows for large time steps without stability losses. While the basic scheme is obtained for the codimension-1, evolutive Mean Curvature Motion, we also present a time-adaptive, a stationary and a codimension-2 version. Numerical tests on classical front evolution benchmarks will also be shown.

Evolutions by crystalline mean curvature. **Antonin Chambolle** (École Polytechnique, France) IC/MT1558/025

I will discuss some recent results, obtained in collaboration with G. Bellettini, V. Caselles, M. Novaga, on the crystalline mean curvature flow of surfaces. These include existence and uniqueness of convex flows, existence of convex flows with forcing term, including with constant volume, convergence to regular flows of (crystalline) "diffusion-generated" motions, implicit discretization by a variational approach (following Almgren-Taylor-Wang's or Luckhaus-Sturzenhecker's ideas) and numerical implementation by combinatorial optimization techniques (in collaboration with J. Darbon).

IC/MP107/025: Recent advances in front propagation modelling and applications. #2

Organiser: Maurizio Falcone (Universita' di Roma "La Sapienza", Italy)
Co-organiser: Regis Monneau (Ecole Nationale des Ponts et Chaussées, France)

(For abstract, see session #1 above.)

Very-weak solutions for a dislocation dynamics model. **Pierre Cardaliaguet** (Université Brest, France) IC/MT1458/025

In some models of dislocation dynamics one is lead to solve an Eikonal equation involving a (non-monotone) non-local term. Existence of classical viscosity solutions for such an equation is not known in general. In this joint work with G. Barles, O. Ley and R. Monneau we investigate a notion of very weak solution for such a model. We prove the existence of these solutions and show that they coincide with the classical viscosity solutions in cases where these latter are known to exist.

A generalized fast marching method applied to dislocations dynamics. **Elisabetta Carlini** (Università degli Studi di Roma "La Sapienza", Italy), Maurizio Falcone (Universita' di Roma "La Sapienza", Italy), Regis Monneau (Ecole Nationale des Ponts et Chaussées, France) IC/MT3373/025

We study dislocation dynamics with a level set point of view. The model represents a dislocation in a 2D plane by the zero level set of the solution of a non local and non convex eikonal equation. We first present a new Fast Marching algorithm for a non-convex eikonal equation modeling front evolutions in the normal direction. The algorithm is a generalization of the Fast Marching Method since the new scheme can deal with a *time-dependent* velocity without *any restriction on its sign*. We prove its convergence in the class of discontinuous viscosity solutions. We then extend the algorithm to evolutions with non local speed and we present some numerical simulations of fronts propagating in $\mathbb{R}^2$ applied to dislocations dynamics. Joint work with: M. Falcone, N. Forcadel, R. Monneau.

Recent advances in the level-set method for shape and topology optimization. **Francois Jouve** (Université Paris VII, France), Grégoire Allaire (École Polytechnique Palaiseau, France) IC/MT3783/025

Since the seminal papers in the early 2000s, there has been a burst of publications on the application of the level set method to shape and topology optimization of structures. Most of the recent papers focus on numerical issues for improving the level set method but do not extend so much its range of applicability. Let us mention, for example, works on its coupling with the topological gradient for holes nucleation or velocity/derivative regularization. Most of these recent works consider only compliance optimization which is a notably simpler problem than optimization of a general objective function.

We propose to extend the range of objective functions which are successfully treated by the level set method, and more specifically to treat the case of objective functions depending on the stress tensor. Together with our previous works (eigenvalue and multiple loads optimization, nonlinear elasticity problems, robust or worst-case optimization) it clearly demonstrates that the level set method is a versatile tool for structural optimization which can tackle industrial, and not merely academic, problems.

Front propagation in inverse problems and imaging. **Martin Burger** (Universität Münster, Germany) IC/MT1154/025

In this talk we shall discuss some (mainly nonlocal) front propagation problems arising in the solution of shape reconstruction and segmentation problems. It has become a popular solution method in the last years to construct solution schemes by propagation fronts along negative shape gradients of associated objective functionals. We shall discuss some practical and theoretical issues related to this approach.

In addition we shall comment on the need of additional nucleation mechanisms, e,g. forced by topological derivatives, in order to reach global minima of the objective functionals.

IC/MP117/002: Applications and numerical approximations of geometric partial differential equations.

Organiser: Xiaobing Feng (University of Tennessee, USA)
Co-organiser: Andreas Prohl (Eberhard Karls Universität Tübingen, Germany)

The aim of this minisymposium is to bring together some of world leading active researchers in the area of numerical geometric partial differential equations to present, communicate, and discuss recent developments and advances in numerical methods and simulations of geometric PDEs. Emphases will be given on the algorithmic development, numerical analysis, and emerging applications.
Topics to be covered in the minisymposium are:

1. Development and analysis of efficient discretization methods for geometric PDEs;
2. Development and analysis of fast converging adaptive solution algorithms;
3. Simulations of formations of singularities and continuation past singularities.
4. Applications of geometric PDEs in physics, biology, materials and image science.

Some adaptive methods in geometric analysis and physics. **Michael Holst** (University of California, San Diego, USA) IC/MT3428/025

There is currently tremendous interest in geometric flows due in part to the Ricci flow program in geometric analysis and in part to the recent construction of gravitational wave detectors around the world. In this lecture, we consider some nonlinear stationary and evolution systems arising in Einstein flow. We develop some basic estimates for one of these systems, and then derive *a priori* and *a posteriori* error estimates for Petrov–Galerkin methods. We develop some nonlinear approximation algorithms based on error indicator-driven adaptive methods, and outline some results on convergence and complexity. We illustrate some of the techniques with examples using the Finite Element ToolKit (FETK).

Retrieving topological information from the phase-field description of geometric evolution. **Qiang Du** (Pennsylvania State University, USA) IC/MT3671/025

Phase field and diffuse interface are popular methods for the modeling and simulations of evolving interfaces. They do not track the interface explicitly, and are insensitive to topological events. In some areas of applications, detecting and controlling topological change may be important. In this talk, we discuss some recent works with colleagues at Penn State on the development of effective formula for retrieving topological information within the phase field framework.

Gradient flows for shape optimization and applications. **Ricardo Nochetto** (University of Maryland, USA) IC/MT3726/025

We present a variational framework for shape optimization problems that hinges on devising energy decreasing flows based on shape differential calculus followed by suitable space and time discretizations (discrete gradient flows). A key ingredient is the flexibility in choosing appropriate descent directions by varying the scalar products, used for computation of normal velocity, on the deformable domain boundary. We discuss applications to image segmentation, optimal shape design for PDE, and surface diffusion, along with several simulations exhibiting large deformations as well as pinching and topological changes in finite time. This work is joint with E. Baensch, G. Dogan, P. Morin, and M. Verani.

A level-set approach to anisotropic flows with curvature regularization. **Frank Haußer** (FZ caesar, Germany), Axel Voigt (FZ caesar, Germany), Martin Burger (Universität Münster, Germany), Christina Stöcker (FZ caesar, Germany) IC/MT3604/025

Modeling and simulation of faceting effects on surfaces are topics of growing importance in modern nanotechnology. Such effects pose various theoretical and computational challenges, since they are caused by non-convex surface energies, which lead to ill-posed evolution equations for the surfaces. In order to overcome the ill-posedness, regularization of the energy by a curvature-dependent term has become a standard approach, which seems to be related to the actual physics, too. The use of curvature-dependent energies yields higher order partial differential equations for surface variables, whose numerical solution is a very challenging task.

In this paper we investigate the numerical simulation of anisotropic growth with curvature-dependent energy by level set methods, which yield flexible and robust surface representations. We consider the two dominating growth modes, namely attachment-detachment kinetics and surface diffusion. The level set formulations are given in terms of metric gradient flows, which are discretized by finite element methods in space and in a semi-implicit way as local variational problems in time. Finally, the constructed level set methods are applied to the simulation of faceting of embedded surfaces and thin films.

IC/MP117/002: Applications and numerical approximations of geometric partial differential equations. #2

Organiser: Xiaobing Feng (University of Tennessee, USA)
Co-organiser: Andreas Prohl (Eberhard Karls Universität Tübingen, Germany)

(For abstract, see session #1 above.)

Convergence of discrete schemes for the Perona–Malik equation. **Giovanni Bellettini** (Dipartimento di Matematica, Universita' di Roma To, Italy) IC/MT2712/025

We discuss the convergence of the spatial semi-discrete scheme for the one-dimensional Perona–Malik equation $u_t = (\phi'(u_x))_x$, $\phi(p) := \frac{1}{2}\log(1+p^2)$, when the initial datum $\overline{u}$ is 1-Lipschitz out of a finite number of jump points, and also in the more difficult case when $\overline{u}$ has a whole interval where $\phi''(\overline{u}_x)$ is negative. In the latter case, the limit solution u we obtain is the same as the one obtained by replacing $\phi(\cdot)$ with the truncated function $\min(\phi(\cdot),1)$, and it turns out that u solves a free boundary problem. Finally, we consider the limits of the full space-time discretization (implicit in time) of the Perona-Malik equation. Work in collaboration with M. Novaga (Dipartimento di Matematica, Università di Pisa, Largo B. Pontecorvo 5, 56127 Pisa, Italy, E-mail: novaga@dm.unipi.it), M. Paolini (Dipartimento di Matematica e Fisica, Università Cattolica di Brescia, via Trieste 41, 25121 Brescia, Italy, E-mail: paolini@dmf.unicatt.it) and C. Tornese (Dipartimento di Matematica, Università di Roma "Tor Vergata", via della Ricerca Scientifica, 00133 Roma, Italy, E-mail: tornese@mat.uniroma2.it).

Combination of global and local approximation schemes for harmonic maps. **Sören Bartels** (Humboldt-Universität zu Berlin, Germany) IC/MT3308/025

It is well understood that a good way to discretize a pointwise length constraint in partial differential equations or variational problems is to impose it at the nodes of a triangulation that defines a lowest order finite element space. In this talk we pursue this approach and discuss the iterative solution of the resulting discrete nonlinear system of equations for the simplest model problem that defines harmonic maps into spheres. An iterative scheme that is globally convergent and energy decreasing but slowly convergent is combined with a locally, rapidly convergent approximation scheme. An explicit example proves that the local approach alone may lead to ill-posed problems; numerical experiments show that it may actually diverge or lead to highly irregular solutions with large energy if the starting value is not chosen carefully. A combination of the global and local method defines a reliable algorithm that performs very efficiently in practice and provides numerical approximations with bounded energy.

A finite-element method for Landau–Lifschitz equations. **François Alouges** (Université Paris-Sud, France) IC/MT3738/025

The behavior of the magnetization inside a ferromagnetic body is modelized by the Landau–Lifchitz equations. These equations write down as a non-linear, slightly dissipative, partial differential equation whose unknown is the magnetization, a 3 dimensional vectorfield which is assumed to be of constant magnitude throughout the body. When one wants to solve numerically these equations, one usually faces the problem of taking into account the (non-convex) constraint that the magnetization belongs to the unit sphere $\mathbb{S}^2$ of $\mathbb{R}^3$ at every point. Besides that, it is of high importance for real applications that the scheme does not produce too much artificial viscosity and is also consistent with the original problem. Writing finite element schemes in that framework - though not obvious - is also challenging because the shapes of the objects that physiscists consider may be (and actually are) arbitrary.

In this talk, we will present some of the latest results, both analytical and numerical, in that direction focusing on the interaction between the nonlinearity due to the constraint and the terms in the equation which come from the model.

Recent developments on numerical methods for second-order fully-nonlinear PDEs. **Xiaobing Feng** (University of Tennessee, USA) IC/MT1977/025

In this talk, I shall discuss some recent developments on numerical approximations of 2rd order fully nonlinear PDEs. The focus of the talk will be on presenting a newly developed vanishing moment method and the notion of moment solutions for 2rd order fully nonlinear PDEs and on discussing the convergence of the method and the relationship between moment solutions and viscosity solutions. The vanishing moment method combined with existing wealthy numerical methods/algorithms for high order quasilinear PDEs makes it possible to construct practical and convergent numerical methods for computing moment and viscosity solutions of 2rd order fully nonlinear PDEs, a task which was largely untouchable before. I shall also present some numerical experiment results for the Monge-Ampere equation, the Gauss curvature equation, and the infinite Laplace equation to demonstrate both convergence and efficiency of the vanishing moment methodology for solving 2rd order fully nonlinear PDEs.

This is a joint work with Michael Neilan of the University of Tennessee, U.S.A.

IC/MP37/025: Modeling and numerical methods for multi-dimensional and multi-physical problems.

Organiser: Juergen Geiser (Humboldt-Universität zu Berlin, Germany)

The motivation for this mini-symposium came from the need to solve complex physical based models. The amount of new methods has increased in the last years but a simplification should took place to solve the complicate models. Complicated models in material and environmental science are possible to solve with such discretisation and solver methods, that are parallel and adaptive. Because of the tremendous interest in climate change, material research and air pollution the development in this direction has increase enormously. These problems are recently actual and interest the people in the western civilization. For such problems a huge class of iterative solver methods are developed. We will focus on advanced discretization and iterative solver methods which are more effective and appropriate to the problems. In this case the class of implicit-explicit and splitting methods could reach a new quality to solve such complicate problems. In the past many software tools have been developed for one-dimensional and simple physical problems; e.g., one-dimensional transport codes or reaction-codes based on ODEs. But the future interests will be coupling of such simple physical and one-dimensional problems to multi-physical and multi-dimensional problems. In this field the coupling of various software tools are interested to simulate the forced complex models. The software recycling and re-engineering of such coupled models will reduce the programming time and lead complex models to adequate applications.

We would like to bring numerical analysts, software developer, modelers, applied engineers and physicists together to discuss methods based on discretization and iterative solver methods for models in solid and fluid mechanics.

Adaptive split schemes for quenching problems. **Qin Sheng** (Baylor University, USA) IC/MT3524/043

This talk concerns certain adaptive finite difference methods for solving multidimensional quenching differential equations,

$$u_t = a^2(u_{xx} + u_{yy}) + \frac{c}{(1-u)^2}.$$

Splitting strategies will be used to achieve the efficiency as well as accuracy of the numerical methods. Analysis on the stability, monotonicity and global error estimates will be given.

Numerical examples will be given to illustrate our results.

Splitting methods for molecule orientations of liquid crystals and liquid-crystal flows. **Ping Lin** (National University of Singapore) IC/MT3279/025

The liquid crystal molecule orientation is arranged by minimizing so-called Oseen–Frank energy functional. The energy is nonconvex due to the unit-length constraint of liquid crystal molecules and the constraint is treated by the penalty method. A time-splitting method is used to compute the solution and its orientation singularities. The liquid crystal flow is a coupling between a director field (molecule orientation) of liquid crystals and a flow field. The model is also related to phase field models of multiphase flows and to microfluidics device. It is crucial to preserve the energy law of the system in numerical simulation, especially when orientation singularities are involved. We present a discrete energy law preserving C0 finite element method. A fixed point iterative method is presented to split the director and flow fields and to achieve a matrix free method in time. A number of liquid crystal and liquid crystal flow examples are computed to demonstrate our algorithms.

Robust error control of Cahn–Hilliard equations with elasticity. **Rüdiger Müller** (Humboldt-Universität zu Berlin, Germany) IC/MT4142/025

Phase separation of an initially homogeneous mixture into different phases can be modeled by the Cahn-Hilliard equation. The interface thickness between the bulk phases enters as a small parameter ϵ into this fourth order semilinear parabolic equation. We also consider the case that elastic stresses due to the lattice misfit become important and the equation has to be coupled to an elliptic system.

When ϵ is very small numerical methods could take great advantage of adaptive mesh refinement that requires error control based on a-posteriori estimators. The numerical analysis of the Cahn-Hilliard equation is well established for fixed parameter size ϵ. But up to now, a-posteriori error estimates depend exponentially on ϵ^{-1} and thus become useless for small ϵ.

In this talk we present an a-posteriori error estimate, that only depends on a low order polynomial of ϵ^{-1}. It is based on the observation that the lowest eigenvalue of the linearized problem is bounded, as long as no topological changes occur. On the other hand, by monitoring this eigenvalue, critical points in the solution can be detected. The results are illustrated with numerical experiments using finite elements and adaptive multigrids.

Description of light focusing by a spherical lens using diffraction integral method. **Shekhar Guha** (Air Force Research Lab., Wright–Patterson AFB, USA), Leonel Gonzalez (General Dynamics Corporation, USA) IC/MT3779/025

A full diffraction theory describing the focusing of light by an arbitrary lens element is not easily available. The complications arise from the inapplicability of the paraxial approximation and the Śthin-lensŠ approximation to the case of light focusing by a general ŚthickŠ lens having a small f-number. When these approximations are not used, the computation time involved in evaluating the diffraction integrals becomes very large for ordinary size lenses (1 cm or larger) for light wavelengths in the visible and infrared wavelengths (400 nm Ű 10000 nm). In this work, we will present the results of application of the Stratton-Chu vector diffraction integrals to a lens having two spherical surfaces, on one of which a plane wave of light is incident. The values of the fields on the second surface and then the field propagated outside the lens will be calculated by repeated use of the diffraction integrals. The limits of computation using current resources will be explored and experimental measurements verifying the calculated results will be presented.

IC/MP223/025: High-resolution discretizations of initial boundary-value problems.

Organiser: Thomas Hagstrom (The University of New Mexico, USA)
Co-organiser: Timothy Warburton (Rice University, USA)

To solve difficult problems in computational science and engineering high-resolution methods allowing a minimal number of degrees-of-freedom per wavelength are required. The difficulty is to effectively apply such methods in complex geometry or for nonlinear problems. The speakers in this minisymposium will discuss a variety of techniques for stably implementing efficient approximation schemes for challenging applications, with a focus on hyperbolic systems of partial differential equations. Examples include high-order discontinuous Galerkin methods on unstructured grids as well as high-order difference approximations on block-structured or purely Cartesian grids with embedded boundaries. Issues to be addressed include:

- The avoidance of excessive time-step stability constraints associated with one-sided approximations or small cells;
- Discrete stability estimates and stability;
- Robust treatment of singularities;
- Exploration of non-polynomial bases;
- Demonstration of serious applications and general-purpose software.

Taming the CFL condition of the discontinuous Galerkin method. **Timothy Warburton** (Rice University, USA) IC/MT3410/025

The upwind discontinuous Galerkin method is an attractive method for solving time-dependent hyperbolic conservation laws. It is possible to use high-order explicit time-stepping methods and high-order spatial approximations without incurring heavy numerical linear algebra overheads. However, the Courant-Friedrichs-Lewy (CFL) condition for these methods depends on the polynomial order used and there is a somewhat excessive cost for using very high order spatial approximation. We will discuss the impact of a staggered grid based filter on the CFL number for these methods and present an algorithm which has CFL number independent of the spatial order of approximation. We will also present computational results for advection, advection-diffusion, and the wave equation on one-dimensional meshes using up to tenth order in space and time.

Finally, we will compare the efficiency of the staggered grid filter with a second approach for taming the CFL condition based on the Koslov/Tal-Ezer mapping technique.

A stable high-order finite-difference scheme for the Navier–Stokes equations. **Jan Nordström** (FOI and Uppsala University, Sweden) IC/MT2206/025

We discuss various aspects of a high order finite difference scheme applied to the Navier-Stokes equations. We discuss the stability obtained by using the concept of summation-by-parts operators in combination with the weak penalty technique for imposing boundary and interface conditions. We adress different aspects of the weak boundary conditions such as accuracy, stability, errorbounds and the reflective/non-reflective properties.

We also show how to construct a stable and accurate hybrid method for nonlinear phenomenona in complex geometries in combination with requirements of accurate signal transportation in domains with smooth flow and geometries. Two separate solvers, one the high order finite difference method discussed above and another using the node-centered unstructured finite volume method is coupled in a truly stable way. The two flow solvers run independently and recieve and send information from each other by using a third coupling code.

The potential of the CELL *processor for improving the numerical efficiency of discontinuous Galerkin methods.* **Jean-François Remacle** (Universite Catholique de Louvain, Belgium) IC/MT3339/025

In this talk, we will present a strategy that enables to solve large scale CFD problems using the new CELL processor.

The new CELL processor combines the considerable floating point resources required for demanding numerical algorithms with a power- efficient software-controlled memory hierarchy. Despite its radical departure from previous mainstream/commodity processor designs, Cell is particularly compelling because it will be produced at such high volumes that it will be cost-competitive with commodity CPUs.

High order Discontinuous Galerkin methods are characterized

by high computational intensity and regular memory access patterns, making them an extremely well suited candidate for the Cell architecture. In a recent work, Williams et al. have used the CELL processor for doing BLAS3 DGEMM matrix-matrix computations. An outstanding performance of about 200 GFlops was observed. We have all the reasons to believe that the CELL and the DGM will be able to develop lots of affinities.

Yet, a main concern of ours is to maintain the memory signature of the method as low as possible while obtaining a quadratic convergence in the resolution of non linear systems. This has led us to develop a Newton-Krylov solver coupled with a p-multigrid preconditionner. The oveall implicit strategy will be given and first computations with the CELL will hopefully presented.

IC/MP223/025: High-resolution discretizations of initial boundary-value problems. #2

Organiser: Thomas Hagstrom (The University of New Mexico, USA)
Co-organiser: Timothy Warburton (Rice University, USA)

(For abstract, see session #1 above.)

Stabilizing high-resolution one-sided difference operators. **Thomas Hagstrom** (The University of New Mexico, USA) IC/MT2715/025

For the numerical simulation of waves, the benefits of high-resolution discretizations with small dispersion errors are clear. However, near physical or element boundaries the direct use of wide-stencil, one-sided formulas whose accuracy matches that of the interior scheme typically leads to instabilities associated with the Runge phenomenon. For polynomial-based pseudospectral methods these instabilities are partially suppressed through the use of an appropriately graded mesh with quadratic clustering near the boundaries. There is still a cost; namely the bounds on the derivative operator grow quadratically with the polynomial degree.

In this talk we focus on the issue of optimal subsampling near the boundary for high-resolution difference formulas. We show experimentally that high-order (up to 22) one-sided difference formulas can be stabilized by the addition of $1-3$ subcell nodes without the excessive growth of the norm of the operator inherent in Chebyshev clustering. We also consider the generalization of the construction to optimized discretizations such as Tam's DRP schemes as well as difference methods built from band-limited bases such as the Knab-Whittaker functions. We present results from experimental codes implementing this construction on overlapping composite grids both for first-order and second-order hyperbolic systems.

A defect of the analysis we have performed so far is that it is almost entirely experimental. We close with some ideas about developing a comprehensive theory of subsampling and extrapolation.

Fast solver for the heat equation in unbounded domains. **Jing Rebecca Li** (INRIA Rocquencourt, France), Leslie Greengard (Courant Institute, NYU, USA) IC/MT2689/025

We describe a fast solver for the inhomogeneous heat equation in unbounded domains. It relies on several new tools: the spectral approximation of the free-space heat kernel, the nonuniform fast Fourier transform, and accurate quadrature methods for the evaluation of heat potentials. Unlike finite difference and finite element techniques, diffusion into an infinite medium is satisfied analytically, avoiding the need for artificial boundary conditions on a finite computational domain. The method is explicit, unconditionally stable, and requires an amount of work of the order O(M N log N) where N is the number of discretization points in physical space and M is the number of time steps.

An example from dendritic solidification will be presented.

Plane-wave approximations for Maxwell's equations in isotropic and anisotropic media. **Tomi Huttunen** (Kuopion Yliopisto, Finland), Peter Monk (University of Delaware, USA) IC/MT2979/025

We investigate the Ultra Weak Variational Formulation (UWVF) of Maxwell's equations for approximating electromagnetic wave fields in isotropic and anisotropic media. We show that the UWVF method can be considered as a Discontinuous Galerkin method when the test functions are local solutions of the Maxwell system. Hence, as proposed by the originators of the UWVF, a linear combination of plane waves can be used for the elementwise approximation of the wave field. However, the number of basis functions for each element must be chosen carefully to avoid ill-conditioning of the resulting matrix equation. Parallelized 3D numerical simulations suggest that the UWVF can successfully simulate wave propagation in isotropic media at relatively high wave numbers. Furthermore, we show that it is possible to extend the method to problems in anisotropic media.

IC/MP276/025: Numerical methods for multicomponent flows.

Organiser: Alexander Kurganov (Tulane University, USA)
Co-organiser: Alina Chertock (North Carolina State University, USA)

Multicomponent flow models arise in many different applications including mixing processes, bubbly flows, liquid suspensions, multilayer shallow water equations, and many others. These models can be divided into two major groups. The first one consists of models where the fluids interface can be practically tracked: a multifluid technique is then applied near the interface only, while away from it a single fluid method(s) can be safely used. When the number of material interfaces increases beyond the practically traceable one, the second group of models is typically used. The equations now describe the fluids mixture, in which all fluid components are assumed to be present and the conservation laws are written for the volume/mass fractions of each phase. No interface tracking is then needed, but the main difficulties are loss of hyperbolicity and/or presence of nonconservative terms that make both analysis and numerical treatment of multiphase models extremely challenging. In the limiting cases, the models from both groups may serve as two possible alternatives to describe the same physical phenomenon.

Development of highly accurate and reliable numerical methods for multicomponent models is of great importance for understanding the aforementioned physical systems. Multifluid numerical algorithms based on a direct extension of single fluid approaches may run into unexpected difficulties due to nonphysical oscillations generated across material interfaces, lack of hyperbolicity and/or a naive discretization of nonconservative terms. Thus, derivation of new genuinely multicom-

ponent techniques is absolutely necessary in the presence of fluid interfaces and interactions between the flow components. In this mini-symposium, speakers will describe their latest progress in development of new numerical methods and improvement of existing ones for both types of the above described models.

Solving the derivative Riemann problem for the Baer–Nunziato equations. **Eleuterio Toro** (Università degli Studi di Torino, Italy) IC/MT3765/025

In this paper we construct semi-analytical solutions to the derivative Riemann problem (DRP) for the Baer–Nunziato (BN) equations for compressible two phase flows. The DRP is the Cauchy problem for the relevant system of equations in which the initial condition consists of two smooth vectors separated by a discontinuity at the origin. The solution, as a function of time, is sought right at the interface. The technique used [1], [2] is an extension of the Cauchy-Kowaleski method and expresses the solution as a power series expansion at the origin. The determination of the leading term requires the solution of a classical Riemann problem for the full BN system. Exact and approximate solvers are discussed for this purpose. The high-order terms require the solution of a sequence of linearized homogeneous Riemann problems for spatial derivatives.

The solutions are systematically assessed against reliable reference solutions obtained numerically. Application of the solutions to construct numerical schemes for solving numerically the general initial-boundary value problem following the ADER approach [3]-[4] for the BN system are also discussed.

Work done in collaboration with Cristobal E Castro.

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[3] Toro E F, Millington R C and Nejad L A M (2001) . Towards Very High-Order Godunov Schemes. In Godunov Methods: Theory and Applications, Edited Review, Toro E F (Editor), Kluwer Academic / Plenum Publishers, pp 905-938, 2001.

[4] Toro E F and Titarev V A (2005). ADER Schemes for Scalar Hyperbolic Conservation Laws in Three Space Dimensions. J. Com. Phys, Vol. 202, pp 196-215, 2005.

Hybrid schemes for flows in porous media. **Smadar Karni** (University of Michigan, Ann Arbor, USA) IC/MT2737/025

The Baer–Nunziato two-phase flow model describes flow over a porous bed. It forms a hyperbolic system which is nonconservative due to porosity changes. If the porosity is contant in each phase, the model reduces to two conservative subsystems separated by an interface across which the porosity changes. Numerical solutions may produce completely non-physical solutions, a failure that is attributed to their inability to preserve the entropy across porosity jumps. We present numerical methods that do not produce entropy across porosity jumps, and illustrate their suitability for computations of two-phase flow in porous media for stationary and moving porosity interfaces.

Interface coupling of different models for multiphase flows. **Nicolas Seguin** (Université Pierre et Marie Curie, France) IC/MT1309/025

We present the coupling of different models for multiphase flows. Several models can be coupled, such that two-velocity systems, drift-flux models and homogeneous models. The coupling of general hyperbolic systems will be presented and several examples of coupling will be studied, including the interaction of pressure waves with the interface of coupling.

Thin-film flow influenced by thermal fluctuations. **Günther Grün** (Universität Erlangen–Nürnberg, Germany) IC/MT4702/025

We will be concerned with the effects thermal fluctuations have on spreading and dewetting of thin liquid films. Starting from the incompressible Navier-Stokes equations with noise, a stochastic fourth-order degenerate parabolic equation for the evolution of the film height can be derived – the stochastic thin-film equation. Besides the usual deterministic terms, it contains multiplicative noise within a convective term. We propose a discretisation scheme and we present integral estimates suggesting the existence of a.s. non-negative solutions. Finally, we give both formal and numerical evidence for our conjecture that thermal fluctuations may resolve discrepancies w.r.t. timescales of dewetting between physical experiments and deterministic numerical simulations. This is joint work with N.Dirr, K.Mecke, M.Rauscher.

IC/MP276/025: Numerical methods for multicomponent flows. #2

Organiser: Alexander Kurganov (Tulane University, USA)
Co-organiser: Alina Chertock (North Carolina State University, USA)

(For abstract, see session #1 above.)

Central-upwind schemes for compressible multi-component fluids. **Alexander Kurganov** (Tulane University, USA) IC/MT3234/025

We focus on development Godunov-type central schemes for hyperbolic systems of conservation and balance laws and on their applications to several multi-component models.

Central schemes are simple, robust, and universal methods for general multi-dimensional systems and they can be applied as a black-box solver to a wide variety of problems arising in many different fields. The simplest central scheme is the celebrated Lax-Friedrichs scheme. It is truly robust, but it suffers from an excessive numerical dissipation. Since the end of 1980, several high-resolution central schemes have been proposed following the pioneering work by Nessyahu and Tadmor. We have been working on development of a subclass of central schemes, the so-called central-upwind schemes, which further reduce numerical dissipation present in central schemes by incorporating some upwinding information. At the same time, central-upwind schemes enjoy the major advantage of central schemes: the use of (approximate) Riemann problem solver is avoided.

Applying central-upwind schemes to multi-component flows requires development and implementation of several numerical techniques specifically designed to track the interface between non-mixing fluids; to extract information from the "mixed" computational cells, where the fluids numerically mix (or to replace the information there with a reliable interpolation); to deal with nonconservative exchange terms, which may cause severe numerical oscillations; and several others. These numerical techniques are crucial for successful application of both central and other finite-volume schemes, and we will discuss them in details.

Interface-tracking method for compressible multifluids. **Alina Chertock** (North Carolina State University, USA), Smadar Karni (University of Michigan, Ann Arbor, USA), Alexander Kurganov (Tulane University, USA) IC/MT2738/025

I will present a new finite-volume method for compressible multi-fluid models, in which the fluids are assumed to be separated by the interface[1]. Away from the interface both fluids are described by the Euler equations of gas dynamics with different equations of state (stiff equations of state allow us to model liquid components of multi-fluids). Switching between the equations of state across interfaces makes designing of stable and highly accurate numerical method quite challenging, since appearance of artificially *mixed* cells may lead to significant pressure oscillations (see, e.g.,[2] and the references therein).

The main idea in designing the proposed method is to allow appearance of the *mixed* cells while avoiding the use of the information from these cells in the evolution of the numerical solution. The method is based on tracking the interface (with the help of the level set, particle method, or any other technique) and using special upwinding procedure for computing the numerical fluxes between the mixed cells and their neighbors. Away form the interfaces, any *regular* numerical flux can be used (we have utilized the second-order central-upwind numerical fluxes). When the interface remains in the same cell after one time step, the evolved solution is oscillation-free. However, when the interface propagates to the neighboring cell, we use another upwinding procedure to replace the value in the *corrupted* cell, while the values of the solution in a new mixed cell are computed from the total mass, momenta and energy conservation requirements.

I will show several one- and two-dimensional examples demonstrating the superior performance of the method: very high resolution of contact/material interfaces and lack of oscillations across them.

[1] Chertock, A., Karni, S. and Kurganov, A.; A Sharp Interface Tracking Method for Compressible Multifluids. submitted.
[2] Abgrall, R. and Karni, S.; Computations of compressible multifluids. J. Comput. Phys., 169 (2001), 594–623.

Central-upwind schemes for two-layer shallow-water equations. **Guergana Petrova** (Texas A&M University, USA), Alexander Kurganov (Tulane University, USA) IC/MT1619/025

We derive a second-order semi-discrete central-upwind scheme for the system of two-layer shallow water equations. We prove that the presented scheme is well-balanced and positivity preserving, that is, the depth of each fluid layer is guaranteed to be nonnegative. We also propose a technique for the treatment of the nonconservative interlayer exchange terms.

Our numerical experiments clearly indicate the sharp resolution of the computed solution, the ability to preserve steady states, and the robustness of the proposed method.

A relaxation–projection method for compressible single phase and multiphase flows. **Richard Saurel** (Université de Provence Aix-Marseille I, France) IC/MT1712/025

The numerical diffusion of interfaces separating compressible fluids involves artificial mixtures for which the determination of the correct thermodynamical state is difficult. By considering such zones as physical multiphase mixtures appropriate hyperbolic models can be derived (Saurel, 2007). These models are non conservative, but shock relations are available (Saurel et al., 2006a). Consequently, exact and approximate Riemann solvers can be derived.

However, the numerical approximation of these models poses extra difficulties. The main one is related to the cell average of non-conservative variables. The Godunov average is shown to result in important inaccuracies. To circumvent this difficulty a new relaxation scheme is built (Saurel et al., 2006b). The cell pressure and volumes fractions are determined by solving a relaxation system involving the various sub-volumes and states present in a cell. These sub-volumes correspond to the distances travelled by the various waves emerging of cell boundaries to the interior of the cell. The interactions between the various non-equilibrium sub-volumes are used to build a relaxation system. Its asymptotic solution provides the cell thermodynamic state. This method is very efficient for interface problems even with very large density and pressure ratios.

Strong shock propagation in multiphase mixtures poses another computational challenge related to the partition of the energy among the various phases. Knowledge of the shock relations and Riemann problem solution is not sufficient with non-conservative systems to guaranty convergence of the solution. Examples and possible solutions will be presented.

[1] Saurel, R. et al.; (2006a) Shock Waves. in press.
[2] Saurel, R. et al.; (2006b) (2006b) JCP, in press.
[3] Saurel, R.; (2007)ICIAM 07 Interface Methods in Multiphase Problems.

IC/MP4420/025: Recent advances in interface methods and applications in multi-phase problems.

Organiser: Zhilin Li (North Carolina State University, USA)
Co-organiser: Xiaolin Li (SUNY at Stony Brook, USA)
Co-organiser: Kazufumi Ito (North Carolina State University, USA)

In this min-symposium, the speakers will present their recent research on numerical methods and application to multi-phase flows. Many scientific and engineering problems require a detailed understanding of physics coupled across a dynamically moving interface separating multi-material or multiphase domains. This minisymposium focus on numerical methods in dealing with such problems. The presentations in this minisymposium will address the propagation of the interface geometry, the coupling across the interface of the interior physics on each side of the interface and the physics at the boundary defined by the moving interface.

A grid-based tracking method for moving interface problems. **Hongkai Zhao** (University of California, Irvine, USA) IC/MT1627/026

I will present a new numerical formulation that combines Eulerian and Lagrangian methods naturally for moving interface problem.

A high-order ENO conservative Lagrangian scheme. **Juan Cheng** (IAPCM, Beijing, PR China) IC/MT1499/026

We present a newly developed Lagrangian scheme for solving Euler equations which is based on high order essentially non-oscillatory (ENO) reconstruction. The scheme is conservative for density, momentum and total energy, maintains formal high order accuracy and can achieve at least second order accuracy with moving and distorted Lagrangian meshes, is essentially non-oscillatory, and has no parameters to be tuned for individual test cases. Comparing with many current Lagrangian schemes, our ENO scheme overcomes some of their disadvantages such as non-conservativity of momentum and total energy, low accuracy, and the existence of parameters which must be adjusted for individual test cases. One and two dimensional numerical results will be given to demonstrate the performance of the scheme in terms of accuracy, resolution for discontinuities, and non-oscillatory properties.

Keywords: Lagrangian scheme; high order accuracy; conservative; ENO reconstruction; Euler equations

Green's function approach for elliptic problems with interfacial discontinuity. **Do Wan Kim** (Hanyang University, Republic of Korea), Sukky Jun (University of Wyoming, USA), Seong-Kwan Park (Yonsei University, Republic of Korea) IC/MT2610/026

Although the elegance of the Green's function has attracted many researchers into the integral equation method for decades, higher dimensional Green's function still remains intricate due to the difficulty in managing the singularity and complex geometry. For example, the Green's functions in 2D and 3D for the Poisson problem have logarithmic and pole singularities, respectively. Furthermore, the Green's function has to satisfy homogeneous boundary condition in the Dirichlet problem, which often becomes a strong restriction on the availability for complex geometries.

In this talk, we present a novel Green's function method to effectively solve the elliptic problems:

$$\nabla \cdot (\kappa \nabla u) = f \quad \text{in } \Omega, u|_{\partial\Omega} = u_B \text{ on } \partial\Omega,$$

which is subjected to the interface conditions

$$\left[\kappa \frac{\partial u}{\partial n}\right]_\Gamma = q_\Gamma, \quad [u] = h_\Gamma,$$

where an inclusion belongs to Ω, the boundary of the inclusion is the interface denoted by Γ, f and κ are bounded functions in space, and both q_Γ and h_Γ represents strengths of the single and double layer sources, respectively.

The key idea of the method is to use 1D Green's function only, even for the above multidimensional problems. It is sufficiently simple to obtain the 1D Green's function for various types of differential operators, and the singularity of the 1D Green's function is so weak enough to be handled. It can thus be applied to problems with complicated geometry such as interfacial discontinuity. In particular, the proposed method is not a differential but an integral scheme, so the stability can be assured. The mathematical error analyses will also be presented for both 1D and 2D elliptic problems.

Accurate numerical interface treatments for multiscale problems. **Thomas Hagstrom** (The University of New Mexico, USA) IC/MT2724/026

In recent years there has been great interest in multiscale computations, which we will take to mean the coupling of very fine scale models in small regions to coarser models in the bulk of the domain. Of fundamental importance for the success of this approach is the accurate exchange of information between the two domains. A number of distinct techniques for dealing with this issue have been proposed and implemented. They range from the derivation and direct implementation of nonlocal conditions, to semilocal approximations based on least squares fitting, to the use of ad hoc damping layers. Our goal in this talk is to review and analyze existing methods in the context of a unified mathematical framework. We will explore the analogies between the multiscale interface problem and the easier problem of radiation boundary conditions for hyperbolic systems. For the latter, an extensive theory exists and a number of very accurate and efficient methods are available. Lastly, we will present some numerical experiments to compare methods and assess the utility of the mathematical theory.

IC/MP4420/025: Recent advances in interface methods and applications in multi-phase problems. #2

Organiser: Zhilin Li (North Carolina State University, USA)
Co-organiser: Xiaolin Li (SUNY at Stony Brook, USA)
Co-organiser: Kazufumi Ito (North Carolina State University, USA)

(For abstract, see session #1 above.)

Adaptive algorithms for phase field models of some interface problems. **Qiang Du** (Pennsylvania State University, USA) IC/MT156/010

We present our on-going works with colleagues at Penn State on the numerical algorithms for the phase field simulations of some interface problems, ranging from microstructure evolution in multicomponent alloy to multicomponent lipid vesicles. We discuss recent development of highly adaptive computational algorithms for large scale phase field simulations. We also address how to effectively retrieve useful statistical information within the phase field framework.

Validation of turbulent-mixing simulations. **James Glimm** (SUNY at Stony Brook, USA) IC/MT415/010

We consider the mixing zone generated by steady acceleration of a fluid interface between two fluids of different densities (Rayleigh-Taylor instability). Recent improvements to the front-tracking algorithm FronTier and to the modeling of transport phenomena in these simulations allows agrement between simulation and experiment for a number of experimental cases. Closures for averaged equation mixing models show good agreement when compared to such direct simulations.

An interoperable front-tracking code and applications to various scientific problems. **Xiaolin Li** (SUNY at Stony Brook, USA), James Glimm (SUNY at Stony Brook, USA) IC/MT1491/026

We introduce an enhanced front tracking method and its software implementation with an easy-to-use user interface. New algorithms include conservative coupling in ND and locally grid based topological bifurcation for 3D. Objective mathematical and computational assessment are given with comparison to other interface methods such as the level set method and volume of fluid method. We emphasize the interoperability of front tracking with other scientific software including the combined operation with AMR and combustion packages. Scientific applications include the study of turbulent mixing due to acceleration driven instabilities, fuel injection jet, shock flame interaction, extending to cell motion in biology. This work is in collaboration with the FronTier Group at Stony Brook University.

Extension of the finite-difference Stokes solvers to irregular domain and two-phase problems. **Vita Rutka** (Universität Konstanz, Germany) IC/MT2576/026

The idea of Immersed Interface Methods (IIM) is to work on grids that do not have to be aligned to possible discontinuities in equation parameters and solution.

The Explicit Jump Immersed Interface Method (EJIIM) [Wiegmann, 1998], is a modification of the original IIM for elliptic partial equations, where the jumps in the unknown function and its Cartesian derivatives are introduced as explicit additional variables into the system. Near discontinuities, the standard numerical method, serving as the basis, is modified by adding correction terms that involve jumps in the function and its derivatives.

In the implementation of the method, the base numerical method, like central finite differences on a regular parallelepiped, can be clearly separated from the EJIIM correction due to the non-grid aligned boundary and/or interface.

We will analyse and compare different finite difference realizations of the Stokes equations coupled with the EJIIM. Issues like staggered versus non-staggered grid or saddle point formulation versus several Poisson problems will be discussed and compared in their performance.

A numerical method for soluble surfactants on moving interfaces. **Shilpa Khatri** (NYU/KTH, USA) IC/MT5058/026

In many real world multiphase flow problems, there are surfactants present. These are surface reacting agents that modify the strength of the surface tension. The concentration of the surfactant on the interface separating the fluids can be modeled with a time-dependent differential equation defined on the time-dependent and deforming interface. For soluble surfactants, this is also coupled to a PDE for the concentration of surfactants in the bulk.

We present a second order method based on an explicit but yet Eulerian discretization of the interface. We use standard finite difference schemes on the discretization of the interface to solve the PDE for the surface concentration. The PDE for the concentration in the bulk will, in the spirit of interface tracking methods, be solved on a fixed uniform grid. The interface arbitrarily cuts through the uniform grid so the boundary flux condition for the bulk surfactant needs a special treatment. We will discuss the details of this implementation and show results in two dimensions.

IC/MP177/025: Solution of the master equation in biochemistry.

Organiser: Per Lötstedt (Uppsala University, Sweden)
Co-organiser: Markus Hegland (Australian National University)

Simulation *in silico* of biological cells is important in the emerging field of systems biology. The macroscopic model equations for simulation of biochemical reactions in the cells are the reaction rate equations. They form a system of deterministic, nonlinear ordinary differential equations for the concentrations of the participating chemical species. This model is accurate for reactions with many participating molecules of each species. If the number of molecules is small or if the reactions occur far from thermodynamic equilibrium, then a stochastic model on a mesoscale such as the chemical master equation is a much more precise description. This is often the case in molecular biology where the majority of the reacting molecules are found in copy numbers less than one hundred in cells such as *Escherichia coli*.

The chemical master equation is a differential–difference equation for the time-dependent probability density of the number of molecules of each participating species. The spatial dimension of the problem is given by the number of species. Since this number may be many thousands in a cell and 10–100 in simpler models, the computational problem using standard methods is enormous with an exponential growth in work and storage with the number of species.

There are different ways of avoiding the *curse of dimensionality*. Sparse grids is a technique for sparse representation of smooth solutions in high dimensions. Gillespie's algorithm is a Monte Carlo method for generating trajectories of the chemical systems and it has been modified to include spatial diffusion. A hybrid method combines the macro and mesoscales and a deterministic algorithm with a Monte Carlo algorithm. These new methods will be described in the minisymposium and applied to many examples from molecular biology including gene regulatory networks.

Multi-scale modelling of biochemical systems by the chemical master equation. **Kevin Burrage** (University of Queensland, Australia) IC/MT1795/025

Biochemical reactions underlying genetic regulation are often modelled as a continuous-time, discrete-state, Markov process, and the evolution of the associated probability density is described by the so-called chemical master equation (CME). However the CME is typically difficult to solve, since the state-space involved can be very large or even countably infinite. Until now this has meant that the direct computation of the probability density function (pdf) associated with chemical kinetics that takes into account intrinsic noise has not been computationally feasible.

Recently a finite state projection method (FSP) that truncates the state-space has been suggested by Munsky and Khammash and shown to be effective on small scale problems. Presented in this talk is a Krylov FSP algorithm based on a combination of state-space truncation and inexact matrix-vector product routines. This allows larger-scale models to be studied and solutions for larger final times to be computed in a realistic execution time.

We compare the efficiency of this technique with trajectorial approaches such as the Stochastic Simulation Algorithm and also show how a strong trajectory can be computed directly from the pdf computed by the CME. Numerical results indicate that this new approach can be fast and is extendable to large biological models.

This is joint work with MARKUS HEGLAND, SHEV MACNAMARA, AND ROGER B. SIDJE

A master equation approach to stochastic reaction diffusion modeling of living cells . **Johan Elf** (Harvard University, USA) IC/MT1450/025

I will discuss how the reaction diffusion master equation [1] can be used to model stochastic reaction diffusion kinetics in intracellular chemical reaction pathways. The exceptionally high dimensionality of the equation makes it practically impossible to solve directly, instead I will describe an efficient Monte Carlo algorithm, the Next Subvolume Method [2], that generates statistically correct trajectories of the stochastic kinetics. Efficient implementation of the algorithm is finicky, why we have developed the MesoRD software [3]. MesoRD can be used to simulate general biochemical reaction networks described in SBML [4] in geometries described by CSG [5]. I will show how we have used MesoRD to understand noise induced ef-

fects in the spatiotemporal fluctuations of the Min proteins in the bacterium *E. coli* [6].

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On the numerical solution of the master equations with sparse grids . **Markus Hegland** (Australian National University) IC/MT186/025

The understanding of complex biological pathways faces the challenge of many randomly interacting components. The evolving probablity distributions describing populations of such systems are modelled by the Chapman/Kolmogorov or chemical master equations. These probability distributions are used to describe the location and range of clusters of the population. They are also used for maximum likelihood methods for the determination of model parameters describing the propensities. However, the representation of these models does have to address the curse of dimensionality. In this talk we will discuss ways how this curse can be dealt with using sparse grid approximation techniques, and, in general, discuss numerical approximations used to solve the chemical master equations.

Hybrid method for the chemical master equation. **Per Lötstedt** (Uppsala University, Sweden) IC/MT1700/025

In the macroscopic model for chemical reactions, the reaction-rate equations are solved for the concentrations of the reacting chemical species. This is a good model if many molecules of each species are present. If there are few molecules of each kind as it often is in a biological cell, then a mesoscopic model including intrinsic noise is much more accurate. The standard method for solution of the mesoscopic master equation is Gillespie's Monte Carlo method. A hybrid method has been constructed combining the best features of both approaches. A stochastic model is introduced only where it makes a difference and the faster solution methods available for the deterministic reaction rate equations are used as much as possible. The reaction rate equations approximate the expected values of the concentrations obtained with the master equation. The expected values of the stochastic variables for the deterministic equations are computed by a quasi-Monte Carlo method. Examples from biochemical systems in molecular biology illustrate the method. This is joint work with Andreas Hellander.

IC/MP310/025: Computational advances in evolving interfaces.

Organiser: Karol Mikula (Slovak University of Technology Bratislava, Slovakia)
Co-organiser: James Sethian (University of California, Berkeley, USA)
Co-organiser: Peter Frolkovič (Universität Heidelberg, Germany)

Dynamic interfaces and moving free boundaries arise in a broad range of applications as material science, structural mechanics, computational fluid dynamics, image processing, computer vision and many others. They represent, e.g., the boundaries between solid and liquid phase in the solidification of materials, boundaries between immiscible liquids in multiphase flows, discontinuities representing edges in digital image segmentation, etc. An interface is represented by a closed curve in 2D or a hypersurface in 3D, and can be advected by an external velocity field and, moreover, its shape can be influenced by a principle of the minimization of surface or elastic energy. Lagrangean, Level-set and Phase-field approaches are well-known computational techniques for approximation of moving interfaces.

The goal of this mini-symposium is to discuss recent computational advances in solving moving free boundary problems, as adaptive high resolution finite element/ finite volume/finite difference solutions on general grids, tangential stabilization of Lagrangean algorithms for evolving curves and surfaces, and other issues important from modeling, implementation and simulation point of view, as well as practical applications where moving interfaces arise.

Evolving curves and sufaces in 2D and 3D image segmentation. **Karol Mikula** (Slovak University of Technology Bratislava, Slovakia) IC/MT2646/025

Evolving curves and surfaces are extensively used in applied sciences and engineering nowadays. In this talk we discuss a Lagrangean and Level-set approaches to solution of the corresponding geometric partial differential equations and the application of the computational methods to 2D and 3D image segmentation problems. In a detail we present semi-implicit complementary volume numerical scheme for solving Riemannian mean curvature flow of graphs and level sets applied to 2D and 3D image segmentation, edge detection, missing boundary completion and subjective contour extraction. We discuss level-set models leading to mean curvature driven image segmentation and outline basic advantages of the so-called subjective surface method given by the solution of the level-set equation

$$u_t = \sqrt{\varepsilon^2 + |\nabla u|^2}\nabla.\left(g(|G * \nabla I^0|)\frac{\nabla u}{\sqrt{\varepsilon^2 + |\nabla u|^2}}\right), \quad (1)$$

where g is nonincreasing (so called Perona-Malik) function, $\varepsilon > 0$ and $G * \nabla I^0$ is a smoothed gradient of the segmented image. We present stability and experimental convergence properties of the method on nontrivial examples of exact solutions and discuss computational results related to biological and medical image segmentation. The given results represent a joined works with Daniel Ševčovič and with S. Corsaro, A. Sarti and F. Sgallari.

Geometrical image segmentation by the Allen–Cahn equation. **Michal Beneš** (Czech Technical University, Prague, Czech Republic) IC/MT3057/025

We present an algorithm of pattern recovery (image segmentation) based on the numerical solution of the Allen-Cahn equation. The approach is usually understood as a regularization of the level-set motion by mean curvature where we impose a special forcing term which lets the initial level set closely surround the pattern of interest. We show basic computational features of the algorithm and demonstrate its function on several artificial as well as real examples.

Inverse problem in seismic imaging. **Maria Cameron** (University of California, Berkeley, USA), Andre Garon (École Polytechnique de Montréal, Canada), James Sethian (University of California, Berkeley, USA) IC/MT2839/025

Imaging of earth regions with nonhorisontal subsurface structures and laterally varying sound speed (seismic velocity) is very difficult. Time migration is a robust and efficient type of seismic imaging which does not require the knowledge of seismic velocities. However, it is adequate only for regions with mild lateral velocity variation. Moreover, time migrated images are obtained in somewhat unintuitive time coordinates. Depth migration is a type of seismic imaging which is adequate for regions with arbitrary lateral velocity variation and produces images in regular Cartesian coordinates. However, its implementation requires knowledge of seismic velocity.

Time migration has an additional output: migration velocities given in time coordinates. The goal of this work is to build an efficient algorithm to:

(a) estimate seismic velocities from migration velocities (then one can use these seismic velocities for obtaining depth migrated earth images);
(b) convert the time migrated images directly to regular Cartesian coordinates.

We established theoretical relations between migration velocities and seismic velocities in 2D and 3D using paraxial ray tracing theory. We formulated an inverse problem of finding seismic velocities from migration velocities and developed two numerical approaches for solving it. These approaches include Dijkstra-like Hamilton–Jacobi solvers for first arrival Eikonal equations and techniques for data smoothing. The outputs of our algorithms are seismic velocities and transition matrices from time coordinates to regular Cartesian coordinates. We tested these approaches on synthetic data examples and applied them to a field data example. We demonstrated that our algorithms give a significantly better estimate of seismic velocities than the Dix inversion which is the standard approach.

Numerical simulation of non-viscous liquid pinch off using a coupled level set-boundary integral method. **Maria Garzon** (Universidad de Oviedo, Spain), James Sethian (University of California, Berkeley, USA) IC/CT4944/025

The pinch off of an inviscid fluid column is described using a potential flow model with capillary forces. The interface velocity is obtained via a Galerkin boundary integral method for the 3D axisymmetric Laplace equation, whereas the interface location and the velocity potential on the free boundary are both approximated using level set type techniques on a fixed domain. The algorithm is validated computing the Rayleigh Taylor instability for liquid columns which provides an analytical solution for short times. The simulations have been continued in time and the algorithm is capable to handle pinch-off and after pinch-off events.

IC/MP310/025: Computational advances in evolving interfaces. #2

Organiser: Karol Mikula (Slovak University of Technology Bratislava, Slovakia)
Co-organiser: James Sethian (University of California, Berkeley, USA)
Co-organiser: Peter Frolkovič (Universität Heidelberg, Germany)

(For abstract, see session #1 above.)

Advances in advancing interfaces: visco-elastic jets and semiconductor manufacturing. **James Sethian** (University of California, Berkeley, USA) IC/MT3065/025

We will describe new applications of interface techniques to problems in manufacturing. In viscoelastic two-phase flow, which is part of pigment-based dyes in ink jet plotters, drug delivery systems, and manufacturing of high resolution display devices, we discuss algorithms based on a combined level set second order projection method for viscoelastic flows with high Weissenberg numbers, showing the effects of viscoelasticity on droplet ejection and dynamics. In semiconductor manufacturing, we discuss problems in superconformal electrodeposition, involving metallization transport and concentration diffusion.

Tangentially stabilized algorithms for evolving curves. **Daniel Ševčovič** (Comenius University, Slovakia) IC/MT1602/025

We study evolution of plane curves satisfying the geometric equation $v = \beta(x, \nu, k, k_{ss})$ where v is the normal velocity, k and ν are the curvature and tangential angle of a plane curve $\Gamma \subset R^2$ at a point $x \in \Gamma$. We follow the so-called direct approach in order to derive a governing system of partial differential equations for the curvature, tangential angle, local length and position vector of the curve. These equations include a nontrivial tangential velocity functional yielding a uniform redistribution of grid points and thus preventing numerically computed solutions from forming various instabilities. We discretize the governing system in order to find a numerical solution for 2D isotropic and anisotropic plane curve evolution, interface motions in thermomechanics and medical image segmentation problems. This is a joint work with K.Mikula. Recent preprints and papers on this topic are available at www.iam.fmph.uniba.sk/institute/sevcovic

On the parametric finite-element approximation of evolving hypersurfaces in $\mathbb{R}^3$. **Robert Nürnberg** (Imperial College London, UK), John Barrett (Imperial College London, UK), Harald Garcke (Universität Regensburg, Germany) IC/MT1567/025

We present a variational formulation of motion by minus the Laplacian of curvature and mean curvature flow, as well as related second and fourth order flows of a closed hypersurface in $\mathbb{R}^3$. On introducing a parametric finite element approximation, we prove stability bounds and compare our scheme with existing approaches. The presented scheme has very good properties with respect to the distribution of mesh points and, if applicable, volume conservation.

Flux-based level set method: finite-volume method for evolving interfaces. **Peter Frolkovič** (Universität Heidelberg, Germany) IC/MT3045/025

The flux-based level set method is a finite volume method for solving an evolving interface implicitly described by a level set function [1]. The motion can be defined by an external passive transport and by a velocity given in the normal direction to the interface that can depend also on the mean curvature.

The level set equation is reformulated to a divergent form with a source term. The advective part is solved using high-resolution flux-based finite volume method [2] that is consistent on unstructured grids and second order accurate for smooth exact solutions. The numerical scheme for the advection is explicit, and the standard CFL restriction on time steps can be removed by using a recursive distribution of fluxes, the so called flux-based method of characteristics [3].

The parabolic part is solved using semi-implicit vertex-centred finite volume method (control volume or co-volume method) that has no restriction on time steps due to stability reasons. The combination of both methods defines the flux-based level set method. The method can be implemented by relatively

small changes to existing codes of finite volume methods for convection-diffusion equations.

Several examples will be given that illustrates the properties of the flux-based level set method like the consistency on locally adapted unstructured grids, second order accuracy for smooth solutions, the first order accuracy (approached from above) in more involved cases, a good behaviour even for largely distorted distance functions, and so on. The presented applications will include the modelling of convection-diffusion in two-phase flows with mass transfer through the interface, the problem of sail-boat distance, and others. The simulations are realized using the free software UG (Unstructured Grids) and the Matlab.

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IC/MP150/025: Time integration of evolution equations.

Organiser: Alexander Ostermann (Universität Innsbruck, Austria)
Co-organiser: Mechthild Thalhammer (Universität Innsbruck, Austria)

Nonlinear evolution equations are fundamental in the description of complex dynamical processes. For the solution of realistic models, due to their complex and possibly chaotic nature, it is indispensable to utilise advanced numerical methods. The main topics of this minisymposium are: geometric integrators, exponential integrators and splitting methods.

In many situations, to obtain more specific information on physically relevant behaviour, it is essential that the numerical method preserves structural properties of the underlying problem. This includes conservation of energy and momentum, positivity, and multi-symplectic structures. In the last years, such geometric integration methods have received a lot of interest.

In connection with structure-preserving time integration methods, exponential integrators are attracting much interest. In contrast to standard integrators, they allow the use of large time-steps for oscillatory problems. Moreover, they have excellent stability properties.

Another topic that will be covered by our minisymposium is the numerical analysis of splitting methods. For problems in many space dimensions, such methods are widely used. Their error behaviour, however, is far from being well understood.

Runge–Kutta convolution quadrature methods for well posed equations with memory. **César Palencia** (Universidad de Valladolid, Spain), Mari Paz Calvo Cabrero (Universidad de Valladolid, Spain), Eduardo Cuesta (Universidad de Valladolid, Spain) IC/MT4033/025

Runge–Kutta based convolution quadrature methods for abstract, well-posed, linear, and homogeneous Volterra equations, non necessarily of sectorial type, are developed. A general representation of the numerical solution in terms of the continuous one is given. The error and stability analysis is based on this representation, which also shows that the numerical solution inherits some interesting qualitative properties, such as positivity, of the exact solution. Numerical illustrations are provided.

Exponential integrators for applications in relativistic laser plasma dynamics. **Marlis Hochbruck** (Universität Düsseldorf, Germany), Julia Schweitzer (Universität Düsseldorf, Germany) IC/MT4013/025

A mathematical model of the interaction of relativistically intense electromagnetic waves with a plasma leads to a system of coupled nonlinear Klein-Gordon equations. The quantities of interest are the vector potential of the laser pulse and the electron density of the plasma. Numerical difficulties of this problem arise because of the oscillatory nature of the solution both in time and space and because of the interest in long-time simulations.

The standard approach for solving these equations numerically is to apply a pseudospectral discretization in space using FFT and to integrate in time with the Störmer/Verlet scheme. In this talk we present an alternative which results in the constructing of a new exponential integrator for this particular application.

This is joint work with Ch. Karle, E.W. Laedke, and K.H. Spatschek, Institute for Theoretical Physics, Heinrich-Heine Universität Düsseldorf.

Understanding the leapfrog scheme via trigonometric integrators. **Christian Lubich** (Universität Tübingen, Germany) IC/MT4986/025

We present results on the long-time near-conservation of energy, momentum and actions in full discretizations of semilinear wave equations in the weakly nonlinear regime. Here we consider pseudospectral discretization in space and the standard leapfrog discretization in time. The results come about by the technique of modulated Fourier expansions and by interpreting the leapfrog method as a trigonometric integrator with modified frequencies. The conservation properties differ markedly from those for standard Runge-Kutta methods.

David Cohen, Ernst Hairer, Christian Lubich, Conservation of energy, momentum and actions in numerical discretizations of nonlinear wave equations, Report, April 2007.

Exponential operator splitting for time-dependent Schrödinger equations. **Mechthild Thalhammer** (Universität Innsbruck, Austria) IC/MT3996/025

In this talk, we consider evolution equations involving an unbounded linear operator. The focus is on problems related to time-dependent Schrödinger equations or spatial discretisations thereof. Our concern is to analyse the convergence and stability behaviour of high-order exponential operator splitting methods. The theoretical error bounds are illustrated by numerical examples.

IC/MP231/025: Numerical methods for option pricing.

Organiser: Olivier Pironneau (Université Paris VI, France)
Co-organiser: Jari Toivanen (Stanford University, USA)

This minisymposium considers deterministic numerical methods for option pricing based on partial (possibly integro) differential equations. Models for underlying assets including jumps lead to non local integral terms. The numerical treatment of these terms is challenging already for low dimensional models. Levy Copulas offer a way to generalize jump models for higher dimensions. When option price depends on more than three factors traditional methods for PDEs are not efficient. Sparse grids give a way to discretize these higher dimensional problems with a feasible amount of unknowns leading to usable methods. For many European options it is possible to derive analytical formulas, but American options lead to nonlinear problems which have to be priced numerically. Lagrange multiplier approach offers a theoretically sound and computationally efficient way to price American options. In order to use the option pricing model in practice, they have to be calibrated using market data, that is, their parameters have to tuned so that that they give prices which match market prices. These calibration problems are typically computationally very challenging and they require efficient methods. All these above mentioned topics are considered in this minisymposium.

Sparse-grid methods for the fast evaluation of financial derivatives. **Michael Griebel** (Universität Bonn, Germany) IC/MT1334/025

We present sparse grid quadrature methods for the evaluation of options and other financial instruments. They are, as MC and QMC methods, able to cope with high(er) dimensional problems. In constrast to MC or QMC these techniques exploit any additional smoothness of the integrand. We consider various applications from finance and discuss the advantages of the sparse grid technique for different financial instruments.

Solving the forward Kolmogorov equation for options in 2D. **Olivier Pironneau** (Université Paris VI, France), Nicolas Lantos (Université Pierre et Marie Curie, France) IC/MT3935/025

Pricing complex options such as baskets or those modeled by stochastic volatilities may involve solving multi-dimensional Black-Scholes like equations. Computing several such options at once can be a numerical challenge. We investigate here the Kolmogorov equation and Dupire or “pre-Dupire" equations to solve the problem faster and validate the approach numerically. The heart of the method is to use the adjoint of the PDE of the option at the discrete level and to use discrete duality identities to obtain Dupre-like relations. The method works on most linear models. Results will be given for basket options and Heston stochastic volatility models and others.

Lagrange-multiplier approach for american options. **Kazufumi Ito** (North Carolina State University, USA) IC/MT2385/025

A general class of parabolic variational inequalities is discussed and the existence and uniqueness of the strong and weak solution are established. Our approach is based on the Lagrange multiplier treatment and the solution is defined as a a unique asymptotic limit of solutions to a family of nonlinear parabolic equations as regularization parameter tending to the infinity. The monotonicity results of the regularized solutions and convergence rate are established. The results are applied to the Black-Sholes model for American option. The case of the bilateral constraint is also treated. A numerical result for the Black-Sholes model is presented and demonstrates a practical usage and interpretation of our results.

High-dimensional PDE methods applied to option pricing. **Yves Achdou** (Université Paris VII, France), Olivier Pironneau (Université Paris VI, France), David Pommier (BNP Paribas France) IC/MT3936/025

Recent developments have shown that it may be possible to use deterministic Galerkin methods or grid based methods for elliptic or parabolic problems in dimension d, for $4 \leq d \leq 20$: these methods are based either on sparse grids [1] or on sparse tensor product approximation spaces [2,3].
Sparse grids were introduced by Zenger [4] in order to reduce the number of degrees of freedom of discrete methods for partial differential equations. Standard piecewise linear approximations need $O(h^{-d})$ degrees of freedom, (h is the mesh step), and produce errors of the order of $O(h^2)$. The piecewise-d-linear sparse grid approximation requires only $O\left(h^{-1}|\log h|^{d-1}\right)$ degrees of freedom, while the error is $O\left(h^2|\log h|^{d-1}\right)$.
We discuss the use of these methods for the numerical solution of diffusion or advection-diffusion problems introduced in option pricing. We consider contracts on multi-assets and European vanilla contract in multifactor stochastic volatility models.

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IC/MP231/025: Numerical methods for option pricing. #2

Organiser: Olivier Pironneau (Université Paris VI, France)
Co-organiser: Jari Toivanen (Stanford University, USA)

(For abstract, see session #1 above.)

Computational methods for Levy models in finance. **Christoph Schwab** (ETH Zürich, Switzerland) IC/MT2132/025

We report on our development of deterministic computational techniques for financial models with jumps. Such models emerged in the past decade as generalizations of the Black-Scholes models, s tarting with the work of Madan and Seneta in 1990. Our approach is based on Galerkin discretizat ion of the process' infinitesimal generator resp. Dirichlet form in a multiscale basis. The meth ods allow to value single and multiperiod contracts, european, american or exotic, on single und erlyings or baskets. Before illustrating the techniques by a number of case studies, among other s for Levy copula dependence models, stochastic volatility models and continuous time GARCH mode ls, we explain the computational techniques and hint at their mathematical background. Determini stic computation of certain optimal hedging strategies by these methods will also be addressed. Joint work of the CMQF group in the Seminar for Applied Mathematics, ETH.

A fast FFT-based method for pricing early-exercise options under Levy processes. **Cornelis Oosterlee** (TU Delft, The Netherlands) IC/MT2126/025

A fast and accurate method for pricing early exercise and certain exotic options in computational finance is presented in this paper. The method is based on a quadrature technique and relies heavily on Fourier transformations. The main idea is to reformulate the well-known risk-neutral valuation formula by recognising that it is a convolution. The resulting convolution is dealt with numerically by using the Fast Fourier Transform (FFT). This novel pricing method, which we dub the Convolution method, CONV method for short, is applicable to a wide variety of payoffs and only requires the knowledge of the characteristic function of the model. As such the method is applicable within exponentially Lévy models, including the exponentially affine jump-diffusion models. For an M-times exercisable Bermudan option, the overall complexity is $O(MN\log(N))$ with N grid points used to discretise the price of the underlying asset. It is shown how to price American options efficiently by applying Richardson extrapolation to the prices of Bermudan options.

A fast and accurate method in pricing early-exercise options under Levy processes. **Fang Fang** (TU Delft, The Netherlands) IC/MT2216/025

When valuing and risk-managing exotic derivatives, practitioners demand fast and accurate prices and sensitivities. Since the models being used in practice are becoming increasingly more complex, efficient methods have to be developed to cope with such models. Aside from non-standard exotic derivatives, plain vanilla options in many stock markets are actually of the American type. As any pricing and risk management system has to be able to calibrate to these plain vanilla options, it is of the utmost importance to be able to value these American options quickly and accurately. A fast and accurate method in pricing early exercise options is developed in this paper, and it is applicable to exponentially affine jump-diffusion models, exponential Lévy models, and variants hereof. In the remainder we will refer to this class of models as the exponentially affine Lévy class. The method relies heavily on the fast Fourier Transform (FFT) algorithm. Early FFT based solution methods were mainly developed in pricing European options, see Heston (1993) and Carr and Madan (1999). Andricopoulos et al. (2002) introduced the quadrature method QUAD, which can be used to value a variety of options with exotic features. It assumes the transition density of the underlying asset is available in closed-form. As in some models only the characteristic function is known, O'Sullivan (2004) combined the early Fourier transform methods with the QUAD method and developed his QUAD-FFT method. The overall computational complexity of his approach is $O(MN^2)$ with M denoting the number of exercise dates and N being the number of points in the asset dimension. This strain of the literature does not seem to have picked up on unpublished work by Reiner (2000), who recognized that, at least for the Black-Scholes model, an option price can be seen as a convolution of the payoff function and the probability density function. This result is well-established for European payoffs, though Reiner demonstrates that the same idea can be used for Bermudan options as well as for weakly path-dependent options such as discretely sampled Asian options, discretely monitored lookbacks and barriers or cliquets. In our work we combine Reiner's ideas with the work of Carr and Madan into what we call the CONV method, which stands for convolution. It utilizes the power of the FFT algorithm as much as possible so that an overall complexity of $O(MN\log(N))$ is achieved.

The basic idea of the CONV method is to start from the risk-neutral valuation formula,

$$\begin{aligned} C(t,x) &= e^{-r\Delta t}\mathbb{E}^{\mathbb{Q}}_{t,S_t}\left[V(t+\Delta t,y)\right] \\ &= e^{-r\Delta t}\int_{-\infty}^{\infty} V(t+\Delta t,y)f(y|x)dy, \end{aligned} \tag{1}$$

where x and y denote the state variables at time t and $t+\Delta t$, respectively, $C(t,x)$ the continuation value of the option at time t, $V(t+\Delta t,y)$ the value of the option at time $t+\Delta t$, $\mathbb{E}^{\mathbb{Q}}_{t,S_t}$ the expectation operator under risk-neutral measure $\mathbb{Q}$, and $f(y|x)$ the conditional density function of y at $t+\Delta t$ given x at t. If the underlying models satisfy $f(y|x)=f(y-x)$, which is the case for e.g. the previously mentioned one-dimensional exponentially affine Lévy models, (1) is thus equivalent to

$$C(t,x) = e^{-r\Delta t}\int_{-\infty}^{\infty} V(t+\Delta t,x+z)f(z)dz, \tag{2}$$

where $z=y-x$. Damping (2) with $e^{\alpha x}$ and then taking the Fourier transform, we have

$$\begin{aligned} \hat{C}(t,\omega) &= \int_{-\infty}^{\infty} e^{i\omega x}\int_{-\infty}^{\infty} e^{\alpha x}V(t+\Delta t,x+z)f(z)dzdx, \\ &= \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} e^{i(\omega-i\alpha)(y-z)}V(t+\Delta t,y)dy\,f(z)dz, \\ &= \underbrace{\int_{-\infty}^{\infty} e^{i(\omega-i\alpha)y}V(t+\Delta t,y)dy}_{\hat{V}_{t+\Delta t}(\omega-i\alpha)}\cdot\underbrace{\int_{-\infty}^{\infty} e^{i(-\omega+i\alpha)z}f(z)dz}_{\phi(-\omega+i\alpha)}, \end{aligned} \tag{3}$$

where $\phi(v)$ denotes the characteristic function of the density $f(z)$. $C(t,x)$ can be recovered by the inverse Fourier transform on (3). When pricing Bermudan options, which will be the focus of this talk, we subsequently apply the early exercise condition:

$$V(t,x)=\max\left(C(t,x),\ \text{payoff}\right), \tag{4}$$

in order to obtain the option value at time t.

The numerical results will include both CPU times and error/convergence measurements in pricing European, Bermandan and American options under geometric Brownian motion (GBM), the Variance Gamma (VG), and the CGMY model, respectively. As an example, to value a 10-time exercisable Bermudan option (under any of the three models), the method takes 0.03 seconds and returns with an error of order 10^{-5}, and a consistent pointwise second-order convergence in log-stock grid width is observed.

Work in collaboration with R. Lord (Modeling and Research, Rabobank International, Utrecht, The Netherlands), C.W. Oosterlee (Delft University of Technology, Delft Institute of Applied Mathematics, Delft, the Netherlands), and F. Bervoets (Modeling and Research, Rabobank International, Utrecht, The Netherlands).

Numerical valuation of options under Kou's model. **Jari Toivanen** (Stanford University, USA) IC/MT972/025

Under Kou's jump-diffusion model the value of a European option satisfies a partial integro-differential equation. Implicit finite difference discretizations are performed on nonuniform space-time grids. For the evalution of the integral term fast recursion formulas are derived leading to optimal computational cost per time step and second-order accuracy in space.

For European options the resulting dense linear problems are solved using a stationary iterative method which requires only a few iterations. For the treatment of the early exercise constraint of American options an operator splitting method and a penalty method are considered.

Numerical experiments demonstrate that accurate option prices can be obtained in a few milliseconds on a PC.

IC/MP213/025: Multiscale porous media: discretizations.

Organiser: Mary Wheeler (University of Texas at Austin, USA)
Co-organiser: Ivan Graham (University of Bath, UK)
Co-organiser: Hector Klie (University of Texas at Austin, USA)

Multiphase flow, transport, and reaction in porous media have important applications in petroleum reservoir engineering and in groundwater flow. These often involve multiphase multiphysics processes across multiple temporal and spatial scales. This minisymposium delves into the state-of-the-art multiscale and physics-preserving numerical algorithms for such porous media phenomena. It is linked to the two other minisymposia: "Multiscale porous media: solvers" and "Multiscale porous media: applications".

Multiscale discretizations for flow, transport and mechanics in porous media. **Mary Wheeler** (University of Texas at Austin, USA) IC/MT3365/025

A fundamental difficulty in understanding and predicting large-scale fluid movements in porous media is that these movements depend upon phenomena that occur on small scales in space and/or time. The differences in scale can be staggering. Aquifers and reservoirs extend for thousands of meters, while their transport properties can vary across centimeters, reflecting the depositional and diagenetic processes that formed the rocks. In turn, transport properties depend on the distribution, correlation and connectivity of micron-sized geometric features, such as pore throats, and on molecular chemical reactions. Seepage and even pumped velocities can be extremely small as compared to the rates of phase changes and chemical reactions. The coupling of flow simulation with mechanical deformations is also important in addressing the response of reservoirs located in structurally weak geologic formations.

We will focus on the mortar mixed finite element method (MMFE) that was first introduced by Arbogast, Cowsar, Wheeler, and Yotov for single phase flow, later extended to multiphase flow by Lu, Pesyznska, Wheeler, and Yotov, and more recently extended, by Wheeler, to transport. The MMFE method is quite general in that it allows for non-matching interfaces and the coupling of different physical processes in a single simulation. This is achieved by decomposing the physical domain into a series of subdomains (blocks) and using independently constructed numerical grids and possibly different discretization techniques in each block. Physically meaningful matching conditions are imposed on block interfaces in a numerically stable and accurate way using mortar finite element spaces. The mortar approach can be viewed as a subgrid or two-scale approach. Moreover, the use of mortars allows one to couple MMFE and discontinuous Galerkin approximations in adjacent subdomains. In this presentation we will discuss theoretical *a priori* and *a posteriori* results, and computational results will be presented.

Well modeling in the multi-scale finite-volume context based on correction functions. **Patrick Jenny** (ETH Zürich, Switzerland) IC/MT1339/025

A numerical reservoir simulator must accurately resolve the length and time scales associated with the complex interactions that take place when several species (components) are transported via multiple fluid phases through a natural geologic formation of large extent. Natural geologic formations often display high variability, complex patterns of spatial correlation, and span a wide spectrum of length scales. For example, the spatial variation of permeability, which is of central importance here, can be quite significant over relatively small distances. The push for more reliable predictions of flow performance has lead to enormous growth in both the geometric complexity and level of detail incorporated in reservoir characterization models. Because of the complex multi-scale nature of the properties, which usually appear as coefficients in the governing equations, modeling of flow in heterogeneous porous media is an ideal target of multi-scale solution techniques. Recently, a multi-scale finite-volume (MSFV) method [1], which employs basis functions, was developed. Since the basis functions are local numerical solutions, they are able to capture the local fine-scale permeability distribution effectively and allow very accurate pressure interpolations between the coarse-grid nodes. For a large variety of difficult multi-phase flow test cases it was shown that the MSFV solutions are in excellent agreement with the corresponding fine-scale results. Later, the method was extended for compressible [2] and gravity driven [3] flow and a well model was incorporated [4]. Here, an alternative way to deal with wells in the MSFV framework is introduced. Opposed to the previously published method, no well domains need to be specified, however, the new approach requires to iterate.

[1] Jenny, P., Lee, S.H. and Tchelepi, H.; Multi-scale finite-volume method for elliptic problems in subsurface flow simulation. Journal of Computational Physics, 187(1), pp.47–67, 2003.
[2] Lunati, I. and Jenny, P.; Multiscale Finite-Volume Method for Compressible Multiphase Flow in Porous Media. Journal of Computational Physics, 216, pp.616–636, 2006.
[3] Lunati, I. and Jenny, P.; Multi-Scale Finite-Volume Method for Density-Driven Flow in Porous Media. Paper submitted to Journal of Computational Geosciences.
[4] Wolfsteiner, C., Lee, S.H. and H. A. Tchelepi; Well modeling in the multiscale finite volume method for subsurface flow simulation. Submitted to Multiscale Model. Simul.

Combining finite volumes and finite elements for non-matching grids. **Martin Vohralík** (Université Pierre et Marie Curie (Paris 6), France) IC/MT1215/025

We propose and analyze a numerical scheme for nonlinear degenerate parabolic convection–diffusion–reaction equations in two or three space dimensions. We use the cell-centered finite volume method on a given grid, which can be nonmatching and can contain nonconvex elements, for all terms except of the diffusion one, which is discretized by the finite element method on a dual conforming simplicial mesh. In this way, the discrete solution is naturally continuous across the interfaces without introducing any supplementary matching conditions as e.g. in the mortar method. The resulting scheme allows to work with inhomogeneous and anisotropic diffusion tensors, is robust, efficient, locally conservative, and stabilized by only adding the minimal numerical diffusion necessary. We prove its convergence in the degenerate parabolic case using *a priori* estimates and the Kolmogorov relative compactness theorem. We then derive *a posteriori* error estimates in the linear case. They are of residual type and we establish them in the energy norm. We prove that they are both reliable and efficient, giving upper and lower bounds on the error, and semi-robust in the sense that the efficiency constant only depends on local variations in the coefficients and becomes optimal as the local Péclet number gets sufficiently small. They are in particular fully computable (all occurring constants are evaluated explicitly), so that they can serve both as indicators for adaptive refinement or for the actual control of the error. We finally illustrate the above results on numerical simulations of the problem of transport of contaminants in porous media.

This work was done in collaboration with Robert Eymard, Université de Marne-la-Vallée, and Danielle Hilhorst, Université de Paris-Sud and CNRS, France.

Mortar methods as multiscale methods. **Ivan Yotov** (University of Pittsburgh, USA), Mary Wheeler (University of Texas at Austin, USA) IC/MT1782/025

We discuss the relationship between mortar finite element methods and multiscale finite element methods. The latter represent the solution as a sum of a coarse scale and a fine scale (subgrid) component and require solving local fine scale problems to compute the multiscale basis functions. Mortar methods with coarse mortar spaces also resolve the solution on the fine scale on each subdomain, but impose continuity conditions on the coarse scale. A domain decomposition algorithm for the algebraic problem requires solving fine scale local problems on each interface iteration. We study the accuracy and efficiency of the mortar multiscale approach in the context of the multipoint flux mixed finite element method.

IC/MP196/026: Challenges for the accurate solution of Laplace eigenvalue and scattering problems.

Organiser: Timo Betcke (University of Manchester, UK)
Co-organiser: Lehel Banjai (Universität Zürich, Switzerland)

Two fundamental problems of wave computations are the Laplace eigenvalue and the scattering problem. Although often different techniques are applied for these two problems the challenges for the solution of them are very similar, such as the right choice of basis functions for an accurate representation of the solution or high frequency computations, which can be regarded as multiscale problems. In this minisymposium we bring together people who are working on the eigenvalue problem and people who are working on the scattering problem to present these challenges and novel solution techniques for them. The presentations involve applications in the quantum physics of chaotic systems, electromagnetic scattering, error estimates and the design of good approximation bases for these problems.

Approximation theory and bases for the Helmholtz equation. **Timo Betcke** (University of Manchester, UK), Alex Barnett (Dartmouth College, USA) IC/MT1483/026

Solutions of the Helmholtz equation in 2D are closely related to holomorphic functions in the complex plane via the so called Vekua operator. We use this theory to review the application of results from complex approximation theory to the design of fast converging approximation bases for the Helmholtz equation. But not only theoretical convergence rates are important in the design of bases. An equally important question is what bases allow well-conditioned representations of solutions of the Helmholtz equation. We discuss results to this effect and present examples involving the eigenvalue problem and the boundary value problem.

The scaling method for high-frequency eigenvalue calculations. **Alex Barnett** (Dartmouth College, USA), Timo Betcke (University of Manchester, UK) IC/MT2451/026

Eigenmode problems appear in acoustics, electromagnetics, and modern applications such as the design of micro-cavity dielectric lasers. When the wavelength is much shorter than the cavity size this becomes a multiscale problem, and boundary methods are needed. I will present an accelerated variant of the method of particular solutions (MPS, a global bassis approximation method) which allows $O(k)$ modes to be calculated in the effort usually required for a single mode, k being the wavenumber. This removes the need for expensive root-searches along the wavenumber axis. Perturbative analysis of the MPS has also led to new eigenvalue error bounds which are $O(k)$ tighter than the classical bounds of Moler-Payne. Finally I will present some work on applying a generalized MPS to locate complex resonance poles of 2D dielectric optical cavities, which connects directly to scattering problems.

High-frequency electromagnetic scattering by convex polygons. **Stephen Langdon** (University of Reading, UK), Simon Chandler-Wilde (University of Reading, UK) IC/MT1768/026

The authors have recently developed a boundary element method for problems of acoustic scattering by sound soft convex polygons for which, by including in the approximation space products of piecewise polynomials supported on a graded mesh with plane wave basis functions, it has been possible to establish a computational cost that depends only logarithmically on the frequency of the incident wave. In this talk we consider the extension of these ideas to electromagnetic scattering problems which in two dimensions can be formulated as Helmholtz problems with transmission boundary conditions. The transmission boundary condition necessitates the solution of the Helmholtz problem on an interior as well as an exterior domain, and thus the problem is significantly more complicated than the corresponding acoustic scattering problem. Some of the issues involved are closely related to those in the Laplace eigenvalue problem.

The effect of a high wave number on numerical schemes for the Helmholtz problem. **Lehel Banjai** (Universität Zürich, Switzerland), Stefan Sauter (Universität Zürich, Switzerland) IC/MT2124/026

The talk will introduce the well-known pollution effect in the FEM when applied to high-frequency Helmholtz problems. We mention some possible ways to reduce the pollution errors but also the fact that pollution in FEM in dimensions larger than 1 is unavoidable.
BEM seems to be more robust in this aspect, as has been noticed in numerics for some time. However, until recently, few theoretical results have been available that explain this experimentally noted behaviour. For scattering by some special domains (sphere, plane), we give the complete analysis of the Galerkin method. Further, we summarize the known wave number explicit estimates for more general domains.

IC/MP71/026: High-order compact schemes for partial differential equations.

Organiser: Murli Gupta (The George Washington University, USA)

This minisymposium will bring together researchers who have been developing, and testing, high accuracy compact finite difference schemes for the solution of a variety of partial differential equations. Emphasis will be on the use of highly efficient solution techniques such as multigrid and parallel computations, and applications to fluid flow problems. We will invite researchers doing theoretical as well as computational analysis. One of the aims of this minisymposium is to compare the progress made since ICIAM 2003 in Sydney.

An efficient compact formulation for the transient Navier–Stokes equations in biharmonic form. **Jiten Kalita** (IIT Guwahati, India), Murli Gupta (The George Washington University, USA) IC/MT2492/026

We recently proposed a new paradigm for solving the steady-state two-dimensional (2D) Navier- Stokes (N-S) equations using a streamfunction- velocity (ψ-v) formulation. This formulation was shown to avoid the difficulties associated with the traditional formulations (primitive variables, and streamfunction-vorticity formulations). The new formulation was found to be second order accurate, and was found to yield accurate solutions of a number of fluid flow problems.

In this paper, we propose a second order time and space accurate, implicit, unconditionally stable scheme on compact uniform grids for the unsteady incompressible N-S equations based upon the ψ-v formulation. The scheme is used to solve several fluid flow problems, including the flow decayed by viscosity problem, a problem with non-homogeneous source term, both of which have analytical solutions, and, the lid-driven square cavity problem. For the first two problems, our coarse grid transient solutions for high Reynolds numbers (Re) are extremely close to the analytical ones. For the cavity problem, our time-marching steady-state solutions up to $Re = 7500$ are excellent match with established numerical results, and for $Re = 10000$, our study asserts that the asymptotic stable solution is mainly periodic as had been found by some recent studies.

Recent advancements to the generalized high-order compact scheme. **William Spotz** (Sandia National Laboratories, USA) IC/MT3371/026

The generalized high-order compact scheme (GHOC) generalizes the high-order compact (HOC) scheme by applying it to unstructured grids. This is done in a manner analogous to the generalized finite difference method (GFDM), which generates a small linear system for each grid point and its surrounding stencil based on Taylor Series expansions. Numerically inverting this small system yields finite difference approximations to various derivatives at the given point. In the GHOC scheme, this linear system is expanded by including derivatives of the governing equation, and yields higher-order approximations to more derivatives at the central grid point of the stencil. This approach also greatly simplifies the derivation of HOC schemes, as much of the error-prone algebra is now replaced by the numerical inversion of a small linear system. It also provides a elegant framework for handling more complex types of boundary conditions. At the previous ICIAM, I presented analysis and results for the GHOC scheme in 1D. More recent advancements include explorations in 2D, issues regarding reproducing classic HOC results, and more sophisticated error analysis.

On the choice of initial conditions of difference schemes for parabolic equations. **Murli Gupta** (The George Washington University, USA), Manana Mirianashvili (Georgian Academy of Sciences), Givi Berikelashvili (A.Razmadze Mathematical Institute, Georgia) IC/MT3769/026

As a model problem we consider the first initial-boundary value problem for linear second-order parabolic equations with constant coefficients in the domain $Q = \Omega\times(0,T] = (0,1)^2\times(0,T]$:

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} - au + f(x,y,t) \ \text{ in } \ Q$$
$$u(x,y,0) = u_0(x,y) \ \text{ on } \ \Omega, \quad u(x,y,t) = 0 \ \text{ on } \ \partial\Omega\times[0,T].$$

We suppose that the generalized solution of this belongs to the anisotropic Sobolev space $W_2^{s,s/2}(Q)$, $s > 1$.

In the case of difference schemes constructed for this problem, when obtaining convergence rate estimate, compatible with smoothness of the solution, various authors make an assumption that the solution of the problem can be extended to the domain $(-d, 1+d)^2 \times (-d, T]$, with $d > 0$, preserving the Sobolev class.

Investigations have shown that if instead of an exact function $u_0(x,y)$, its approximation (using the above) is taken as an initial condition, then this restriction can be removed.

A high-order alternating direction implicit (ADI) difference scheme is constructed in the paper for which the convergence rate estimate

$$\|\tilde{u} - u\|_{L_2(Q_{h,\tau})} \le C(h^s + \tau^{s/2})\|u\|_{W_2^{s,s/2}(Q)}, \quad s \in (2,4]$$

is obtained. Here $\tilde{u}$ is a solution of the difference scheme, $Q_{h,\tau}$ is a mesh in Q, C is a positive constant independent of h, τ and u, and h and τ are space and time steps respectively.

High-order ADI method for stream-function vorticity equations. **Samir Karaa** (Sultan Qaboos University, Oman) IC/MT3753/026

Many recent works have demonstrated the efficiency of high-order compact difference schemes on the streamfunction and vorticity formulation of 2-D incompressible Navier-Stokes equations. High order compact discretizations induce cross spatial derivatives which are treated explicitly in most ADI schemes. Recently, Karaa and Zhang proposed a fourth order ADI method for solving convection-diffusion problems efficiently. In this work, we extend this method to the solution of incompressible Navier-Stokes equations. Numerical results are obtained for the model problem of driven cavity flow and compared with other results available in the literature.

IC/MP205/026: FETI, balancing, and related hybrid domain-decomposition methods.

Organiser: Axel Klawonn (Universität Duisburg-Essen, Germany)
Co-organiser: Ulrich Langer (Universität Linz, Austria)
Co-organiser: Barbara Wohlmuth (Universität Stuttgart, Germany)

Domain decomposition methods are a successful approach for the solution of the often very large systems arising from the discretization of partial differential equations. The best algorithms from this class of methods are highly scalable on massively parallel computers.

Finite Element Tearing and Interconnecting (FETI) and Balancing Domain Decomposition methods are two related families of such iterative substructuring algorithms which are by now quite well-known. In this minsymposium we gather several active researchers in the field who are going to present their latest results on new theoretical developments, different discretizations and applications, and parallel scalability.

Coupled finite and boundary-element domain decomposition methods. **Olaf Steinbach** (TU Graz, Austria) IC/MT2969/026

Finite and boundary element methods often have complementary properties in different situations. Domain decomposition methods allow to use the discretization method which is the most appropriate one for the subdomain under consideration. The coupling is based on appropriate transmission conditions in which the Dirichlet to Neumann and the Neumann to Dirichlet map play an important role, respectively. Here we give a general overview on different formulations leading to coupled finite and boundary element methods. In general, we have to solve large scale systems of coupled finite and boundary element equations. The efficiency of iterative methods heavily depends on the availability of efficient preconditioners. We consider various solution strategies, in particular tearing and interconnecting methods, and provide appropriate precondi-

tioners resulting in asymptotically almost optimal solvers. This talk summarizes joint work with W. L. Wendland, G. Of, and U. Langer.

Coupled FETI/BETI solvers for nonlinear potential problems in unbounded domains. **Clemens Pechstein** (Universität Linz, Austria), Ulrich Langer (Universität Linz, Austria) IC/MT1828/026

This contribution deals with the numerical solution of nonlinear potential equations of the form $-\nabla \cdot [\nu(x,|\nabla u(x)|)\,\nabla u(x)] = f(x)$, for $x \in \mathbb{R}^d = \overline{\Omega} \cup \overline{\Omega}^c$, where Ω is open and bounded, and $\Omega^c := \mathbb{R}^d \setminus \overline{\Omega}$. Such equations arise e. g. in two-dimensional magnetic field computations. On the unbounded exterior domain Ω^c we assume that $f \equiv 0$ and $\nu \equiv \nu_0 = \text{const}$, and furthermore that $u(x)$ satisfies a suitable radiation condition for $|x| \to \infty$. We apply Newton's method to the nonlinear variational formulation and solve the linearized problems using a special coupled Finite and Boundary Element Tearing and Interconnecting (FETI/BETI) method. In order to get a good initial guess for Newton's iteration, we use the nested iteration strategy based on a hierarchy of nested grids. In case of a nonlinear coefficient, the spectrum of the corresponding subdomain Jacobi matrices may show high variation. In magnetostatic applications, this variation indeed appears in ferromagnetic materials, where the ratio between the largest and the smallest ocurring value of the reluctivity ν can be 10^3 and more. However, the local anisotropy is typically small and the coefficient field has some smoothness properties. We propose a special FETI/BETI preconditioner that shows only a weak dependence of the number of PCG iterations on the variation in our numerical experiments.

For a piecewise constant coefficient, the condition number of the preconditioned FETI/BETI system corresponding to a boundary value problem on Ω is known to be $\mathcal{O}((1+\log(\frac{H}{h}))^2)$, independent of the mesh size h, the maximal edge/face diameter H and possible jumps in the coefficient across subdomain interfaces. Including the exterior space Ω^c as a subdomain, we can show the same estimate if a primal coarse space is chosen accordingly to the FETI-DP variant.

Domain-decomposition multiscale methods for flow in porous media. **Mary Wheeler** (University of Texas at Austin, USA) IC/MT3849/026

A fundamental difficulty in understanding and predicting large-scale fluid movements in porous media is that these movements depend upon phenomena occuring on small scales in space and/or time. The differences in scale can be staggering. Aquifers and reservoirs extend for thousands of meters, while their transport properties can vary across centimeters, reflecting the depositional and diagenetic processes that formed the rocks. In turn, transport properties depend on the distribution, correlation and connectivity of micron sized geometric features such as pore throats, and on molecular chemical reactions. Seepage and even pumped velocities can be extremely small compared to the rates of phase changes and chemical reactions.

We will focus on the mortar methods which was first introduced by Arbogast, Cowsar, Wheeler, and Yotov for mixed finite element method (MFE) approximations for single phase flow and later extended to multiphase flow by Lu, Pesyznska, Wheeler, and Yotov. This method is quite general in that it allows for non-matching interfaces and the coupling of different physical processes in a single simulation. This is achieved by decomposing the physical domain into a series of subdomains (blocks) and using independently constructed numerical grids and possibly different discretization techniques in each block. Physically meaningful matching conditions are imposed on block interfaces in a numerically stable and accurate way using mortar finite element spaces. This domain decomposition approach can be viewed as a subgrid or two scale approach. Moreover, the use of mortars allows one to couple MFE and discontinuous Galerkin approximations in adjacent subdomains. In this presentation we will discuss theoretical *a priori* and *a posteriori* results and computational results will be presented.

Multilevel BDDC. **Bedřich Sousedík** (University of Colorado, USA), Jan Mandel (University of Colorado at Denver, USA), Clark Dohrmann (Sandia National Laboratories, USA) IC/MT3026/026

We present the formulation and condition number bounds for a multilevel version of the BDDC algorithm. The condition number bounds grows polylogarithmically with the ratio of the substructure sizes between levels, but they grow exponentially with the number of levels. Numerical results show that this may indeed occur.

The condition number bounds are based on an abstract multilevel algebraic theory suitable for nested substructuring methods.

IC/MP205/026: FETI, balancing, and related hybrid domain-decomposition methods. #2

Organiser: Axel Klawonn (Universität Duisburg-Essen, Germany)
Co-organiser: Ulrich Langer (Universität Linz, Austria)
Co-organiser: Barbara Wohlmuth (Universität Stuttgart, Germany)

(For abstract, see session #1 above.)

Large-scale simulations of arterial walls: parallel solution strategies. **Oliver Rheinbach** (Universität Duisburg-Essen, Germany), Axel Klawonn (Universität Duisburg-Essen, Germany), Jörg Schröder (Universität Duisburg-Essen, Germany), Dominik Brands (Universität Duisburg-Essen, Germany) IC/MT3577/026

Nonoverlapping domain decomposition methods are fast parallel solvers for large equation systems arising from the discretization of partial differential equations. In this talk, dual iterative substructuring methods of the FETI-DP (Finite Element Tearing and Interconnecting Dual-Primal) type are described and applied to the biomechanical problem of elastic deformations of arterial walls. This problem poses various challenges to solver algorithms (i.e., nonlinearity, almost incompressibility, very large material jumps); e.g., when atherosclerotic plaques with calcifications are present, and anisotropy. Our goal is the developement of a method which performs robustly within this setting and still shows good scalability. The mechanical modeling is the focus of a companion talk by D. Brands.

Extending domain decomposition to problems with irregular subdomains. **Olof Widlund** (Courant Institute, NYU, USA) IC/MT3572/026

In the theory of iterative substructuring methods and certain other domain decomposition algorithms, each subdomain is typically assumed to be the union of a small set of coarse triangles or tetrahedra. Such an assumption is often unrealistic, in particular, if the subdomains are produced using mesh partitioner software. An extension of the theory requires that a number of technical tools be generalized. A survey will be given of recent results.

Optimal TOTAL FETI solver for 3D frictionless-contact problems. **Zdeněk Dostál** (TU Ostrava, Czech Republic) IC/MT3332/026

We shall first briefly review the FETI based domain decomposition methodology adapted to the solution of frictionless multibody contact problems in 3D. We use modification that we call TFETI (Total FETI) [1] which imposes prescribed displacements by Lagrange multipliers. As a result, we shall obtain a convex quadratic programming problem with a special inequality and equality constraints. The classical results concerning the solution of linear elliptic boundary value problems give that the condition number of the Hessian of the quadratic form is bounded independently on the discretization parameter h.

Then we shall present our algorithms for the solution of resulting quadratic programming problems. The unique feature of these algorithms is their capability to solve the class of quadratic programming problems with spectrum in a given positive interval in O(1) iterations. The algorithms enjoy the rate of convergence that is independent of conditioning of constraints and the results are valid even for linearly dependent equality constraints.

Finally we put together our results on approximation of variational inequalities and those on quadratic programming to develop algorithms for the solution of both coercive and semicoercive variational inequalities and show that the algorithms are scalable [2]. We give results of numerical experiments with parallel solution of both coercive and semicoercive problems to demonstrate numerically scalability of the algorithms presented that was predicted by the theory.

The research was carried out in collaboration with my colleagues V. Vondrák and D. Horák.

[1] Z. Dostál, D. Horák and R. Kučera *Total FETI - an easier implementable variant of the FETI method for numerical solution of elliptic PDE*, to appear in Communications in Numerical Methods in Engineering.

[2] Z. Dostál and D. Horák *Theoretically supported scalable FETI for numerical solution of variational inequalities*, To appear in SIAM Journal on Numerical Analysis.

Scalable algorithm for solving 3D contact problems with friction. **Radek Kučera** (TU Ostrava, Czech Republic) IC/MT1926/026

The contribution deals with solving of contact problems with Coulomb friction for a system of 3D elastic bodies. First we introduce auxiliary problem with given friction defining a mapping Φ which associates with a given slip bound the normal contact stress in the equilibrium state. The solution to the contact problem with Coulomb friction is characterized by a fixed point of Φ and the method of successive approximations is used for its computation.

The finite element discretization of the contact problem with given friction leads to constrained minimization of a nonsmooth functional. After using the duality theory, the problem can be rewritten as minimization of a strictly convex quadratic functional with separable convex constraints. To compute the solution we can use a newly developed active-set based algorithm (QPC) that combines the conjugate gradient method with the gradient projections. This algorithm has the rate of convegence in terms of the spectral condition number of the Hessian matrix.

The FETI domain decomposition method impose, in addition, the linear equality constraints in the algebraic formulation of the problem. In order to satisfy them, the iterative augmented Lagrangian algorithm can be used, in which the outer loop updates the Lagrange multipliers for the equality constraints, while the inner loop is represented by the QPC algorithm. Moreover, the update rule for the penalty parameter is introduced that depends on the increase of the augmented Lagrangian.

The main goal is to extend theoretical results obtained recently for 2D contact problems. In particular, it can be proved that if the algorithm is applied to the class of problems with uniformly bounded spectrum of the Hessian matrix, then the algorithm finds an approximate solution at $O(1)$ matrix-vector multiplications.

IC/MP108/010: Interface methods and applications in multi-phase problems.

Organiser: Zhilin Li (North Carolina State University, USA)
Co-organiser: Xiaolin Li (SUNY at Stony Brook, USA)
Co-organiser: Kazufumi Ito (North Carolina State University, USA)

Many scientific and engineering problems require a detailed understanding of physics coupled across a dynamically moving interface separating multi-material or multiphase domains. This minisymposium focus on numerical methods in dealing with such problems. The presentations in this minisymposium will address the propagation of the interface geometry, the coupling across the interface of the interior physics on each side of the interface and the physics at the boundary defined by the moving interface.

Fast locally-corrected boundary-integral methods for elliptic systems. **John Strain** (University of California, Berkeley, USA) IC/MT1363/026

Classical potential theory converts linear constant-coefficient elliptic problems in complex domains into integral equations on interfaces, and generates robust, efficient numerical methods. The conversion is usually carried out for a particular situation such as the Poisson equation in dimension 2, and the efficiency of the resulting methods then depends on detailed analysis of the appropriate special functions.

We present a general conversion scheme which leads naturally to a fast general algorithm: arbitrary elliptic problems in arbitrary dimension are converted to first-order systems, a periodic fundamental solution is mollified for convergence, and the mollification is locally corrected via Ewald summation. Local linear algebra and the elementary theory of distributions yield a simple boundary integral equation. With the aid of a new nonequidistant fast Fourier transform for piecewise polynomial functions, the resulting numerical methods provide highly accurate solutions to general elliptic systems in complex domains.

The augmented immersed-interface method for Stokes and Navier–Stokes equations with interfaces/irregular domains. **Zhilin Li** (North Carolina State University, USA) IC/MT1812/026

The Immersed Interface Method (IIM) was motivated by the Peskin's Immersed Boundary Method. The IIM shares many characteristics of the IB method. Both methods use simple grid structure. The original motivation of IIM is to improve the accuracy of the IB method from first order to second order. This has been achieved by incorporating the jump conditions into numerical schemes near or on the interface. In this talk, I will focus on some recent work using IIM to solve incompressible Stokes and Navier Stokes equations with singular sources and discontinuous viscosity. One of techniques if the augmented approach in which fast Poisson solvers can be used. In the augmented approach, we introduce augmented variables so that the jump conditions for the velocity and the pressure can be decoupled, and the fast Poisson solvers can be employed even though the viscosity is discontinuous. We will also discuss this approach for flows on irregular domains. Numerical examples will also be presented.

An accurate Lagrange multiplier finite element method for interface problems. **Rachid Touzani** (Université Clermont-Ferrand, France), Gunther Peichl (Universität Graz, Austria) IC/MT1596/026

We consider the numerical solution of some elliptic interface problems. Such problems involve the same type of singularities that appear in interface and free boundary problems. For such problems, we design a new finite element method that avoid using fitted meshes. Using a hybrid technique localized at interface elements and a Lagrange multiplier, we construct a finite element that enjoys optimal convergence rates. Numerical experiments confirm the theoretical ones.

Simulating flow around solid body using immersed boundary method. **Lai Ming-Chih** (National Chiao Tung University, Taiwan) IC/MT1505/026

A new immersed boundary (IB) technique for the simulation of flow interacting with solid boundary is presented. The present formulation employs a mixture of Eulerian and Lagrangian variables, where the solid boundary is represented by discrete Lagrangian markers embedding in and exerting forces to the Eulerian fluid domain. The interactions between the Lagrangian markers and the fluid variables are linked by a simple discretized delta function. Based on the direct momentum forcing on the Eulerian grids, a new interpolating force formulation on the Lagrangian marker is proposed, which ensures the satisfaction of the no-slip boundary condition on the immersed boundary in the intermediate time step. This forcing procedure involves solving a banded linear system of equations whose unknowns consist of the boundary forces on the Lagrangian markers; thus, the order of the unknowns is one-dimensional lower than the fluid variables. Four different test problems have been compared with previous experimental and numerical results.

IC/MP108/010: Interface methods and applications in multi-phase problems. #2

Organiser: Zhilin Li (North Carolina State University, USA)
Co-organiser: Xiaolin Li (SUNY at Stony Brook, USA)
Co-organiser: Kazufumi Ito (North Carolina State University, USA)

(For abstract, see session #1 above.)

Multiphase flow theory of diffuse interfaces and transformation fronts. **Richard Saurel** (Université de Provence Aix-Marseille I, France) IC/MT1705/026

The numerical smearing of interfaces separating compressible fluids involves artificial mixing zones for which determination of the correct thermodynamic state is difficult.By considering such zones as physical multiphase mixtures reliable modelling is possible. The non-equilibrium multiphase flow model of Baer and Nunziato (1986) is considered. It is reduced to the single velocity and single pressure but multi-temperatures flow model of Kapila et al. (2001). This model is examined for the modelling of diffuse interfaces separating compressible fluids. This non-conservative hyperbolic model with five partial differential equations requires shock relations for its closure. The shock relations derived in Saurel et al. (2006a) are summarised. Then, extensions to extra physics are considered.

First, capillary effects at interfaces separating compressible fluids are introduced. A conservative formulation is obtained (Perigaud and Saurel (2005)). Second, heat and mass transfer at interfaces are introduced in order to deal with phase transition fronts (Saurel et al., 2006b). When the interface structure is numerically solved evaporation jump conditions are recovered. In particular, the kinetic CJ relation proposed by Simoes Moreira and Shepherd (1999) for evaporation fronts in metastable liquids is obtained as an eigenvalue of the limit system with stiff thermal and chemical relaxation. Examples for multidimensionnal cavitating flows are presented.

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[6] Saurel, R.; (2007) ICIAM 07 Num. Meth. Multicomp. Fl. Also, JCP, in press.
[7] Simoes-Moreira, J.R. and Shepherd, J.E.; (1999) JFM 382: 63-86.

Compact fourth-order finite-difference schemes for elliptic systems and interface problems. **Kazufumi Ito** (North Carolina State University, USA) IC/MT2489/026

Compact fourth-order Cartesian grid-based finite-difference methods are developed for Stokes systems and elliptic interface problems. The resulting system has the $M-$matrix property and thus satisfies the discrete maximum principle. Our methods are based on the continuation of solution across the interface using multi-variable Taylor's expansion of the solution about selected interface points and a set of appropriate interface conditions. The interface conditions are derived from the continuity of the solution and its flux and equating the equation and its derivatives. The method is also successfully extended to the heat equation. The validity and effectiveness of the proposed methods are demonstrated through our numerical results

A coupled IIM–BEM numerical method for the simulation of cell motion in single-cell traps. **Boo Khoo** (National University of Singapore) IC/MT2059/026

We present a coupled Immersed Interface Method–Boundary Element Method (IIM-BEM) numerical technique that can study the (dynamic) behavior of target cells in detail, and describe the cell deformation and motion under the effects of both the electric and the (hydrodynamic) flow fields. We apply this technique to analyze the characteristics of a hybrid electrical-mechanical trap for single-cell trapping in the presence of a cavity on a channel wall. The Immersed Interface Method provides the means of calculating the hydrodynamic effects and influence of fluid-structure interaction such as cell movement and deformation next to the cavity wall, and the Boundary Element Method is used to calculate the electric fields and their effects on the particle. We report on the effect of different combinations of electrode positions and mechanical properties of the trap on the maximum loading and unloading Reynolds numbers, and further show the effect that cells moving with the flow have on cells which have been already trapped in the cavity.

Keywords: Immersed Interface Method, Boundary Element Method, Navier-Stokes equa-tions, Dielectrophoresis, cell traps.

EJStokes: an explicit jump correction to the fast fictitious-force 3D Stokes solver. **Andreas Wiegmann** (Fraunhofer ITWM, Kaiserslautern, Germany), Liping Cheng (Fraunhofer ITWM, Kaiserslautern, Germany) IC/MT2491/026

Wiegmann [1] described the fast fictitious-force 3D Stokes solver for solving steady Stokes equations of the flows in porous media and geometrically complex materials. It is efficient and fast but implements the boundary conditions in tangential directions a half mesh width away from the correct locations. That is because in a MAC grid, the solid interfaces fall between grid cells for the variables in tangential directions. The method enforces the no-slip boundary conditions a half mesh size inside the interfaces. To achieve higher accuracy, this paper adopts a jump correction scheme. The jump correction is derived by using Taylor expansions at the interface points. The expression of the discretized correction terms shows agreement with analytical formulation of a singular force represented on the surface in Stokes equations. With a fictitious force term in normal direction and a jump correction term in tangential directions expressed as unknown body forces, the fast Fourier solver can still be utilized by extending all variables in the solid voxels. The Schur-complement formulation shows the resulting matrix is not symmetric. However, the jump corrected method obtains more accurate results, which is demonstrated by the Poiseuille flow in a channel and in a circular pipe. The accuracy is also verified by comparing to known analytical/numerical solutions for the example of slow flow through a periodic array of spheres centered in a unit cell.

[1] Andreas Wiegmann, FFF-Stokes: a fast fictitious force 3D Stokes solver, in preparation, Nov 2006.

IC/MP59/026: Partial differential equations and Sobolev gradients.

Organiser: Robert Renka (University of North Texas, USA)
Co-organiser: John Neuberger (University of North Texas, USA)

The Sobolev gradient method is a gradient descent method designed to compute critical points of a discretization of a functional of the form $\phi(u) = \int_\Omega F(Du)$, where D is a differential operator, and u is an element of some Sobolev space for which $F(Du)$ is integrable. The Fr'echet derivative of ϕ at u is uniquely represented by an element of the Sobolev space, termed the Sobolev gradient. The central idea of the method is to use the discretized Sobolev gradient rather than the ordinary Euclidean gradient in a method such as steepest descent for minimizing a discretization of ϕ. The resulting method is one of preconditioned gradient descent with an effective preconditioner that arises in a very natural and elegant manner. While the primary application is numerical solution of nonlinear partial differential equations, the method has been extended to geometric modeling problems, inverse problems, optimal control problems, and image processing problems.

Sobolev gradients: superconductivity and other applications. **John Neuberger** (University of North Texas, USA) IC/MT1506/026

We indicate use of Sobolev gradients for Ginzburg–Landau functionals of superconductivity. We indicate how moats and holes in a superconducting medium energentically attract vortices. Other applicatons are indicated including one to problems in transonic flow. Some convergence results are given. A related result is a new Nash–Moser type inverse theorem.

Work on superconductivity is in collaboration with Robert Renka.

Gradient-flows and gradient-like flows. **Ralph Chill** (Universite Paul Verlaine Metz, France) IC/MT1929/026

The title of this talk could also be: *Gradient flows and gradient-like flows associated with a single energy functional.* We will in fact first review that given an energy functional such as the classical functional

$$E(u) := \tfrac{1}{2}\int_\Omega |\nabla u|^2 + \int_\Omega F(u)$$

defined on $H^1_0(\Omega)$ ($\Omega \subset \mathbb{R}^n$ open) it is possible and natural to associate *several* gradient flows and gradient-like flows, usually partial differential equations. It is remarkable that all these flows have similar asymptotic behaviour: for example, solutions of the various flows converge to an equilibrium point as soon as E satisfies a gradient inequality. We will discuss a similar program for energy functionals arising in geometric evolution equations and show how a gradient inequality can also be used to prove global existence.

[1] R. Chill; On the Łojasiewicz-Simon gradient inequality, J. Funct. Anal. **201** (2003), 572–601.
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[3] R. Chill, E. Fašangová, and R. Schätzle; Willmore blow-ups are never compact. In preparation (2006).

Neuberger gradient method applied to design of martensitic microvalves. **Sultan Sial** (Lahore Inst. Of Management Sciences, Pakistan) IC/MT1355/026

Martensitic materials are of interest since all shape-memory materials are martensitic. The method of Neuberger gradients allows for the efficient optimization of free energy of Ginzburg-Landau type. In this talk the formulation and optimization of a functional related to the design of martensitic microvalves is considered.

Application of the Sobolev steepest descent to hyperbolic Monge–Ampere equations. **Tamani Howard** (University of North Texas, USA) IC/MT1349/026

We will address both numerical and theoretical applications of the Sobolev gradient steepest descent method to some hyperbolic Monge-Ampère equations. In the numerical case, we will disscuss the construction of the discrete Sobolev gradient and present some numerical solutions to the hyperbolic Monge-Ampère equation:

$$det(D^2\ z) = f$$

on [0, 1]2 in the two cases where $f = -1$ and $f = -(1 + z_x^2 + z_y^2)^2$. We will also explore the effect of some imposed boundary conditions on the solutions. Finally, in the theoretical case, we will prove convergence of the continuous Sobolev gradient steepest descent in the Sobolev space $H^{9,2}([0,1]^2)$ to show local existence of solutions to the hyperbolic Monge-Ampère equation $det(D^2\ z) = -1$.

IC/MP59/026: Partial differential equations and Sobolev gradients. #2

Organiser: Robert Renka (University of North Texas, USA)
Co-organiser: John Neuberger (University of North Texas, USA)

(For abstract, see session #1 above.)

Curve-fitting with a Sobolev gradient method. **Robert Renka** (University of North Texas, USA) IC/MT1044/026

Consider the problem of constructing a mathematical representation of a curve that satisfies constraints such as interpolation of specified points. This problem arises frequently in the context of both data fitting and Computer Aided Design. We treat the most general problem: the curve may or may not be constrained to lie in a plane; the constraints may involve specified points, tangent vectors, normal vectors, and/or curvature vectors, periodicity, or nonlinear inequalities representing shape-preservation criteria. Rather than the usual piecewise parametric polynomial (B-spline) or rational (NURB) formulation, we represent the curve by a discrete sequence of vertices along with first, second, and third derivative vectors at each vertex, where derivatives are with respect to arc length. This provides third-order geometric continuity and maximizes flexibility with an arbitrarily large number of degrees of freedom. The free parameters are chosen to minimize a fairness measure defined as a weighted sum of curve length, total curvature, and variation of curvature. We thus obtain a very challenging constrained optimization problem for which standard methods are ineffective. A Sobolev gradient method, however, will be shown to be particularly effective.

Image interpolation: a novel variational method. **Santiago Betelu** (University of North Texas, USA) IC/MT1176/026

We study a novel variational method for the interpolation of digital images. In this problem, an image has a region R where the data has been lost or corrupted, and one wants to interpolate this region by using the information from another region M where the image is intact. To formulate the problem, we define a function $u(x, y)$ representing the luminance values of the image, and define an energy E as the integral of a functional $F(u)$ calculated over R. The functional F is estimated from the data in M using probabilistic arguments. The solution of the problem is reduced to a gradient descent minimization of the energy E. Numerous examples are shown and the advantages and disadvantages of the method are discussed.

Uniqueness and reconstruction for the inverse conductivity problem. **Ian Knowles** (University of Alabama, USA) IC/MT2024/026

The inverse conductivity problem centers around the determination of the conductivity p in the conductivity equation $\nabla \cdot (p(x)\nabla u) = 0$ in a region Ω, of dimension two or greater, from a knowledge of the Dirichlet-Neumann mapping Λ_p on the boundary of Ω. We discuss a new method for proving that Λ_p uniquely determines p when p is Lipschitz continuous, as well as steepest descent methods for computing p from Λ_p.

Inverse problems for Maxwell systems. **Malcolm Brown** (Cardiff University, UK), Mohamad Zahran (Hariri Canadian University, Lebanon) IC/MT3667/026

We shall show that the coefficients in the Maxwell system may be recovered from partial boundary data. Theoretical results will be illustrated with numerical examples.

IC/MP265/026: Efficient methods for Hamilton–Jacobi equations.

Organiser: Alexander Vladimirsky (Cornell University, USA)
Co-organiser: James Sethian (University of California, Berkeley, USA)
Co-organiser: Ian Mitchell (University of British Columbia, Canada)

Hamilton–Jacobi equations have natural interpretations in deterministic and stochastic optimal control, differential games, and anisotropic front propagation. Efficient methods for solving these PDEs make useful tools for practitioners in robotics, optimal control, seismology, geophysics, image processing, material science, and financial engineering.

A number of fast schemes were recently introduced for different sub-classes of Hamilton–Jacobi PDEs. The proposed methods reflect a variety of approaches and perspectives (semi-Lagrangian and Eulerian; based on viscosity solutions and on viability kernels; mirroring the properties of label-setting and label-correcting algorithms in the discrete dynamic programming; based on paraxial approximations or on alternating-direction Gauss–Seidel relaxation). This mini-symposium will focus on comparing the efficiency and limitations of these techniques as well as on applicability to other equations and application areas.

Discrete network flows and continuous PDEs: new applications and new Dijkstra-like methods. **James Sethian** (University of California, Berkeley, USA) IC/MT3059/026

Fast Marching Methods are part of a class of Dijkstra-like methods for solving the Eikonal equation. Using this as a starting point, the author will discuss some applications that straddle the boundary between discrete network flow problems and continuous Hamilton-Jacobi equations. Numerous new applications will be presented, including optimal solutions of geodesics on complex terrain.

Fast sweeping methods for convex Hamilton–Jacobi equations. **Hongkai Zhao** (University of California, Irvine, USA) IC/MT1629/026

I will first give a general review for the fast sweeping method, the algorithm, convergence, error estimate and optimal complexity for Eikonal equations. Then I will talk about our recent work (joint work with J. Qian and Y. Zhang) on fast sweeping method for general convex Hamilton-Jacobi equations on unstructured mesh. Finally I will show applications of fast sweeping strategy to other hyperbolic or hyperbolic dominant problems.

Wide-stencil schemes for second-order degenerate elliptic PDEs. **Adam Oberman** (Simon Fraser University, Canada) IC/MT1092/026

The theory of viscosity solutions gives powerful existence, uniqueness and stability results for first- and second-order degenerate elliptic partial differential equations. The approximation theory developed by Barles and Sougandis in the early nineties gave conditions for the convergence of numerical schemes.

While there has been a lot of work on first-order equations, there has been very little work on genuinely nonlinear or degenerate second-order equations. This despite the fact that many of these equations are of the subject of current research and applications. For example: level-set motion by mean curvature, the Infinity Laplacian, the PDE for the value function in Stochastic Control, the Monge–Ampère equation.

In this talk, we build convergent schemes for the aforementioned equations, and also for some less well-known or newer equations, including the Pucci Equations and a new PDE for the convex envelope. We will also discuss a general framework for building these types of schemes. The majority of the work discussed can be found on the author's webpage.

Approximation of solutions to Burger's, Lighthil–Whitham–Richards' and Moskowitz HJB equation. **Patrick Saint-Pierre** (Université Paris Dauphine, France) IC/MT1114/026

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IC/MP265/026: Efficient methods for Hamilton–Jacobi equations. #2

Organiser: Alexander Vladimirsky (Cornell University, USA)
Co-organiser: James Sethian (University of California, Berkeley, USA)
Co-organiser: Ian Mitchell (University of British Columbia, Canada)

(For abstract, see session #1 above.)

Ordered upwind methods for Hamilton–Jacobi PDEs. **Alexander Vladimirsky** (Cornell University, USA) IC/MT2991/026

In discrete-state-space optimal control problems (e.g., shortest-path problems on graphs), the dynamic programming approach yields a large coupled system of non-linear equations. To solve this system efficiently, label-setting algorithms (e.g., Dijkstra's and Dial's methods) re-order the computations and provide an upper bound K on the number of times a single equation has to be solved. The efficiency stems from the fact that K is independent of the total number of equations and of the costs/penalties assigned to the edges of the graph.

Ordered Upwind Methods (OUMs) exploit similar ideas to solve systems arising from causal discretizations of static Hamilton–Jacobi PDEs. We will describe a method for producing causal discretizations, comparing the different effects of Hamiltonian non-convexity, anisotropy and inhomogeneity on the method's accuracy and computational complexity. We will illustrate our method with several examples from optimal control, differential games, and front propagation.

Fast marching and semi-Lagrangian schemes for convex and non-convex Hamilton–Jacobi equations. **Maurizio Falcone** (Universita' di Roma "La Sapienza", Italy) IC/MT2506/026

The talk presents recent results on the approximation of convex and non convex Hamilton-Jacobi equations via semi-Lagrangian approximation schemes. We will examine a Fast Marching semi-Lagrangian approximation for eikonal type equations as well as efficient approximation schemes for non convex Hamiltonians. Several applications to control and game problems, optimal path finding and image processing will be presented.

Works in collaboration with E. Cristiani.

An efficient algorithm to solve perturbed shortest path problems. **Lars Grüne** (Universität Bayreuth, Germany), Oliver Junge (TU München, Germany), Marcus von Lossow (Universität Bayreuth, Germany) IC/MT1541/026

Perturbed shortest path problems form a class of discrete time dynamic games which arise, for instance, from the semi-discretization of Hamilton–Jacobi–Isaacs equations related to pursuit–evasion games or robust stabilization problems. In this talk we present an algorithm for the solution of such problems on a finite state space, along with a set oriented discretization technique which allows to approximate a problem on a continuous state space by problems on finite spaces.

Unlike most efficient computational methods for optimal control problems, which are not easily adapted to the dynamic game setting, here we will show that one of the fastest known methods for shortest path problems, Dijkstra's algorithm, can be extended to a "min–max Dijkstra" algorithm with only moderate increase in the computational complexity. We will discuss the basic idea of this extension as well as implementational aspects. Furthermore we show how a judicious interplay between the set oriented discretization and the min–max Dijkstra algorithm can be used in order to compute upper and lower approximations to the game's value function, a feature particularly useful for suboptimal feedback synthesis.

The proposed method will be illustrated by a number of numerical examples.

Theoretical and experimental results on the complexity of schemes for anisotropic Hamilton–Jacobi equations. **Ian Mitchell** (University of British Columbia, Canada) IC/MT1639/026

The stationary (or static or time-independent) Hamilton-Jacobi equation arises in optimal path planning through continuous domains. In this talk we examine the anisotropic case, where the cost to traverse the path may depend on the direction of travel as well as the states visited. Both iterative and non-iterative schemes are considered, and some conclusions are drawn about the types of grids and cost functions for which various schemes are more or less effective.

IC/MP203/026: Least-squares finite-element methods for partial differential equations.

Organiser: Chad Westphal (Wabash College, USA)

The least-squares approach to numerically approximating the solution to partial differential equations (PDEs) is a powerful methodology that offers several distinctive features not present in more traditional methods. In its simplest form, a least-squares norm minimization principle is applied to the residual of an appropriate first-order system of PDEs, resulting in a symmetric variational problem which is discretized in a finite element context. This allows complete flexibility in choosing finite element spaces for the unknowns, provides a reliable error estimator and leads to naturally positive definite linear algebraic systems that can often be solved with optimal complexity by multilevel iterative solvers.
This approach combines many ideas from the optimization and numerical PDE communities to solve difficult problems. The least-squares methodology puts significant emphasis on development of the original PDE system rather than the discretization or solver. Thus, in general, the key to success lies in choosing the right first-order system and norm in which to minimize over. Often, but not always, this formulation involves introducing new unknowns and additional, but consistent, equations to the system.
In recent years researchers have made great progress toward developing robust solution strategies for a growing number of applications. This minisymposium promises to highlight several challenging nonlinear problems in solid and fluid mechanics which have only recently been analyzed in a least-squares framework. Also of significance in this session are computational advances in h and p refinement techniques and treatment of problems with significant nonlinearities and singularities.

A least-squares finite-element method for visco-elastic fluid flow. **Chad Westphal** (Wabash College, USA) IC/MT1322/026

Viscoelastic materials are those with properties of both viscous fluids and elastic solids. With applications ranging from biological fluids to liquid crystal flows, these models are of general interest to many fields. While much progress has been made in recent years toward the accurate and efficient computational solution of equations for viscoelastic fluids, many difficultes persist. In this talk we present a least-squares finite element method for the steady Oldroyd type viscoelastic fluids. The least-squares methodology offers many attractive benefits which are particularly advantageous for this system. A weighted-norm approach is used to remove effects of corner singularities and a nonlinear nested iteration is used to reduce the overall computational work as well as to ensure good initial guesses for the nonlinear iteration. We also establish equivalence of the homogenous least-squares functional to a meaningful norm, ensuring well posedness of the numerical method in a small parameter regime. Numerical results are given for benchmark problems and large scale flow features are compared with well-known results.

Adaptive local-refinement strategy for FOSLS finite-element method. **Joshua Nolting** (University of Colorado at Boulder, USA) IC/MT1624/026

Adaptive local refinement enables us to concentrate computational resources in areas that need special attention, for example, near steep gradients and singularities. The Least-Squares Finite Element method FOSLS (First Order System Least Squares), yields a very sharp *a posteriori* error measure for each element. This is a benefit that is very important for adaptive refinement strategies, because determining what elements need to be refined, often relies on the measured error for each element. This talk will discuss a strategy for determining which elements to refine in order to optimize the accuracy/computational cost. Set in the context of a full multigrid algorithm, our strategy leads to a refinement pattern with nearly equal error on each element. Further refinement is essentially uniform, which allows for an efficient parallel implementation. Numerical experiments will be presented.

First-order-system least-squares for elasto-plasticity. **Gerhard Starke** (Universität Hannover, Germany) IC/MT1903/026

A least-squares mixed finite element method for the incremental formulation of elasto-plasticity using a plastic flow rule of von Mises type with isotropic hardening is presented. This approach is based on the use of the stress tensor, in addition to the displacement field, as independent process variables. The nonlinear least-squares functional is shown to constitute an *a posteriori* error estimator on which an adaptive refinement strategy may be based. For the finite element implementation under plane strain conditions, quadratic (i.e., next-to-lowest order) Raviart-Thomas elements are used for the stress approximation while the displacement is represented by standard quadratic conforming elements. The method constitutes an extension of a least-squares mixed finite element approach for linear elasticity recently studied in joint work with Zhiqiang Cai and Johannes Korsawe.
Our main theoretical result is that, under the assumption of a plastic flow rule of von Mises type with isotropic hardening, the nonlinear least-squares functional associated with elasto-plasticity is elliptic with respect to an appropriate product space for the stresses and displacements.

Computational results for a benchmark problem of elasto-plasticity under plane strain conditions are presented in order to illustrate the effectiveness of the least-squares approach. Our computational results also suggest that the approximation properties actually deteriorate in the perfectly plastic case. Despite this deterioration of the approximation order in the perfectly plastic case, the adaptive implementation of the least-squares finite element method provides remarkably accurate results, in particular for the stresses.

First-order system least-squares methods for the Signorini contact problem in linear elasticity. **Frank Attia** (Universität Hannover, Germany), Gerhard Starke (Universität Hannover, Germany) IC/MT2687/026

A first-order system least squares formulation for the Signorini problem modelling frictionless contact in linear elasticity is studied. The displacement field and the stress tensor are used as independent process variables. To treat the boundary conditions, appropriate boundary functionals are part of the least squares functional. Coercivity and continuity of this functional allow to use the functional as an *a posteriori* error estimator, which will be used as a basis for an adaptive refinement strategy. For the displacement field, conforming quadratic elements (P2) or non-conforming Mardal-Tai-Winther elements (MTW) can be used. Note that the MTW elements lead to uniform approximation properties for nearly incompressible materials. Computational results for a test problem of Hertzian contact will be shown.

IC/MP258/026: Advances in discontinuous Galerkin methods.

Organiser: Thomas Wihler (McGill University, Canada)
Co-organiser: Ilaria Perugia (Università degli Studi di Pavia, Italy)

Discontinuous Galerkin (DG) finite element methods have gained considerable interest in recent years. The remarkable research activity in this area results, amongst other reasons, from a number of interesting features of DG schemes, which are appealing from both an analytical and computational view point. The goal of this minisymposium is to focus on: new results for DG discretizations in solid and fluid mechanics, and electromagnetics; error analysis; *a posteriori* error estimation and adaptivity; time-dependent problems; high-order DG methods; nonlinear PDE.

Adaptive DG methods for the Stokes problem. **Ohannes Karakashian** (University of Tennessee, USA) IC/MT3507/026

We present some recent results on DG methods for the Stokes problem including lower and upper *a posteriori* error bounds in the energy norm and convergence results for adaptive schemes based on the *a posteriori* bounds.

Hybridized globally divergence-free LDG methods for the Stokes problem. **Dominik Schötzau** (University of British Columbia, Canada) IC/MT2764/026

We devise and analyze a new local discontinuous Galerkin (LDG) method for the Stokes equations of incompressible fluid flow. This optimally convergent method is obtained by using an LDG method to discretize a vorticity-velocity formulation of the Stokes equations and by applying a new hybridization to the resulting discretization. One of the main features of the hybridized method is that it provides a globally divergence-free approximate velocity without having to construct globally divergence-free finite dimensional spaces; only element-wise divergence-free basis functions are used. Another important feature is that it has significantly less degrees of freedom than all other LDG methods in the current literature; in particular, the approximation to the pressure is only defined on the faces of the elements. On the other hand, we show that, as expected, the condition number of the Schur-complement matrix for this approximate pressure is of order h^{-2} in the mesh size h. Finally, we present numerical experiments that confirm the sharpness of our theoretical *a priori* error estimates.

Discontinuous Galerkin methods for anisotropic and possibly locally nondefinite diffusion with advection. **Alexandre Ern** (École Nationale des Ponts et Chaussées, France), Daniele Antonio Di Pietro (École Nationale des Ponts et Chaussées, France), Jean-Luc Guermond (Texas A&M University, USA) IC/MT1297/026

In the present work we construct and analyze a Discontinuous Galerkin method to solve advection-diffusion PDEs with anisotropic and possibly locally nondefinite diffusion. The method is designed so as to automatically detect the so-called elliptic-hyperbolic interface without requiring any further intervention. The key to the method is the use of weighted average and jump operators. The error analysis provides optimal estimates in the broken graph norm and is consistent with well-known results when the problem is either hyperbolic or uniformly elliptic. The theoretical results are supported by numerical evidence.

hp-adaptive discontinuous Galerkin methods for the shallow-water equations. **Clint Dawson** (University of Texas at Austin, USA), Ethan Kubatko (University of Texas at Austin, USA), Joannes Westerink (University of Notre Dame, USA) IC/MT3823/026

The shallow water equations model highly nonlinear hydrodynamic phenomena. The hydrodynamics are driven by tide, winds and waves, gravity, Coriolis and other forces. Typical domains include deeper waters transitioning to continental shelves and shallow coastal regions. Solutions to these models exhibit complex, multiscale spatial and temporal behavior. Dynamically adaptive finite element methods including discontinuous Galerkin methods are currently being pursued for these models. DG methods are of particular interest, because of their ability to handle local h- and p-adaptivity, local mass conservation, and ability to model both smooth and rough flow. In this talk, we will discuss recent advances in the development and analysis of DG methods for the shallow water equations, with applications to flows in inlets, estuaries, and storm surges along the Gulf Coast of the U.S.

IC/MP258/026: Advances in discontinuous Galerkin methods. #2

Organiser: Thomas Wihler (McGill University, Canada)
Co-organiser: Ilaria Perugia (Università degli Studi di Pavia, Italy)

(For abstract, see session #1 above.)

Discontinuous Galerkin finite-element approximation of nonlinear elastic waves. **Endre Süli** (University of Oxford, UK) IC/MT1617/026

We survey recent developments concerned with the construction and convergence analysis of discontinuous Galerkin finite element methods for second-order systems of nonlinear hyperbolic equations of the form

$$\partial_t^2 u_i - \sum_{\alpha=1}^{d} \partial_{x_\alpha} S_{i\alpha}(\nabla u(t,x)) = f_i(t,x), \qquad i = 1,\dots,d,$$

with $\partial_{x_\alpha} = \partial/\partial x_\alpha$, in a bounded spatial domain $\Omega \subset \mathbb{R}^d$, subject to mixed Dirichlet–Neumann boundary conditions. Evolution problems of this kind arise as mathematical models in nonlinear elastic wave propagation.

We first discuss the case when the Piola–Kirchhoff stress tensor $S = (S_{i\alpha})$ is uniformly monotone on $\mathbb{R}^{d\times d}$; the energy functional

$$J : v \mapsto J(v) := \int_\Omega W(\nabla v(x))\,\mathrm{d}x - \int_\Omega f(x)\cdot v(x)\,\mathrm{d}x - \int_{\Gamma_N} g_N(s)\cdot v(s)\,\mathrm{d}s,$$

(where W is the stored energy density function related to S via $S = \nabla W$, $\Gamma_N \subset \partial\Omega$ is the Neumann part of the boundary and g_N is the Neumann boundary datum,) associated with the corresponding static problem

$$-\sum_{\alpha=1}^{d} \partial_{x_\alpha} S_{i\alpha}(\nabla u(x)) = f_i(x), \qquad i = 1,\dots,d,$$

is then convex. Granted sufficient smoothness of u, we show that the discontinuous Galerkin method exhibits an optimal rate of convergence with respect to the spatial discretization parameter.

Using a broken Gårding inequality we extend our convergence results to the case when we only require that the fourth-order elasticity tensor $A = \nabla S$ satisfies a Legendre–Hadamard condition. The associated stored energy density function W is then only rank-1 convex.

The talk is based on joint work with Christoph Ortner (University of Oxford).

Discontinuous Galerkin methods using solutions of the PDE. **Peter Monk** (University of Delaware, USA) IC/MT3588/026

We shall show that a general class of symmetric hyperbolic systems can be discretized using an upwind discontinuous Galerkin method using solutions of the underlying partial differential equation as basis functions for the approximation. With an appropriate choice of degrees of freedom this gives rise to the Ultra Weak Variational Formulation due to Cessenat and Despres.

We shall illustrate this approach with an application to Maxwell's equations, and to the Helmholtz equation. The method is most useful at higher frequencies than is usual for finite element methods, and for moderate accuracy (the conditioning of the system prevents very high accuracy).

We shall present the current state of error analysis of the method using the Helmholtz equation as model problem.

This paper presents joint work with Tomi Huttunen and Matti Malinen from the Department of Applied Physics at the University of Kuopio, Finland.

Multigrid algorithms for some new interior-penalty methods. **Susanne Brenner** (Louisiana State University, USA) IC/MT3485/026

We will discuss multigrid algorithms for some new interior penalty methods. Both convergence analysis and numerical results will be presented.

Discontinuos Galerkin approximation for advection–diffusion–reaction problems. **Blanca Ayuso** (Departamento de Matematicas, Universidad Autonoma, Spain), L. Donatella Marini (Università degli Studi di Pavia, Italy) IC/MT5066/026

In this talk, following the weighted-residual approach recently introduced by Brezzi *et al.* for elliptic problems, we discuss the design of DG approximations for advection–diffusion–reaction problems. We devise the basic ingredients to ensure stability and optimal error estimates in suitable norms, and propose two new methods.

The talk is based on joint work with L. Donatella Marini from the University of Pavia.

IC/MP239/027: Recent advances in algebraic multigrid with applications.

Organiser: Michael Gee (TU München, Germany)
Co-organiser: Marzio Sala (ETH Zürich, Switzerland)

The minisymposium focuses on recent advances in algebraic multigrid methods (AMG) and application of multigrid methods to complex, parallel and large scale applications. While such methods are widely used and accepted for standard applications such as elliptic partial differntial equations, formulation and application of AMG methods to more complex applications such as e.g. multiphysics, fluid dynamics, nonconforming discretizations, anisotropy or Maxwell equations is a very active field of research. The minisymposium provides an overview of current state of the art algebraic multigrid formulations, recent developements and challenging applications. Topics of interest include (but are not restricted to) algebraic multigrid in the context of the following:

- nonlinear multigrid;
- fluid dynamics and multiphysics applications;
- nonsymmetric problems;
- Maxwell equations;
- nonconforming discretizations, constraints and saddle problems;
- adaptive multigrid techniques;
- anisotropic problems and automatic anisotropy detection;
- formulations;
- implementation issues and software engineering;
- scalability;
- algebraic multigrid for matrix-free problems.

Performance of AMG-based preconditioners for fully-coupled Newton–Krylov solution of transport/reaction systems. **John Shadid** (Sandia National Laboratories, USA) IC/MT2572/027

A current challenge before the computational science and numerical mathematics community is the efficient computational solution of multi-physics systems. These systems are strongly coupled, highly nonlinear and characterized by multiple physical phenomena that span a very large range of length and time scales. The myriad of complex, interacting physical mechanisms can balance to produce steady-state behavior, nearly balance to evolve a solution on a dynamical time scale that is long relative to the component time-scales, or they can be systems that are dominated by one (or a few) process(es). These characteristics make the computational solution of these system extremely challenging.

In this presentation I will briefly motivate the need for fully-coupled Newton-based solution techniques for coupled nonlinear multiple-time-scale PDE systems. The resulting large sparse linear systems that are generated by these methods are solved by the application of parallel preconditioned Krylov methods. The preconditioners we consider include additive Schwarz domain decomposition (DD) and multi-level preconditioners. The multi-level preconditioners are based on geometric and algebraic methods as well as approximate block factorization techniques.

To demonstrate the capability of these methods I will present performance results for representative transport/reaction systems such as chemically reacting flows, semiconductor devices and possibly some recent plasma system simulations. In this context I will discuss robustness, efficiency, and the parallel and algorithmic scaling of solution methods.

This work was partially funded by the Department of Energy's Mathematical, Information and Computational Sciences Division, and was carried out at Sandia National Laboratories operated for the U.S. Department of Energy under contract no. DE-ACO4-94AL85000.

Point-based AMG for strongly-coupled PDE systems: recent developments for several industrial applications. **Tanja Clees** (Fraunhofer SCAI, Germany), Peter Thum (Fraunhofer Institute SCAI, Germany), Klaus Stüben (Fraunhofer SCAI, Germany) IC/MT2636/027

Algebraic multigrid (AMG) methods are known to be very efficient and robust solvers or preconditioners for large classes of problems, such as discretized scalar elliptic partial differential equations (PDEs). They can handle millions of variables and are especially suited for unstructured grids. Straightforward extensions of AMG, for example, so-called unknown-based (or function-based) approaches, have successfully been applied to different types of PDE systems. But for other important problems, the usage of more sophisticated methods, for example, so-called point-based approaches, is necessary.

Within the solver library SAMG, developed at Fraunhofer SCAI, a whole framework of point-based approaches has already been realized. The robustness and efficiency of concrete approaches for several practically important classes of applications, for instance, in semiconductor simulation (including strongly coupled drift-diffusion systems), has already been demonstrated.

For some other important application classes, efficient and robust (S)AMG strategies have lately been developed. This includes PDE systems arising in oil reservoir simulation (strongly coupled black oil as well as compositional models; geophysics). For others, promising strategies have recently been designed. Among such application classes are computational fluid dynamics (Navier-Stokes equations) and simulations of electrochemical machining and plating processes (PDE systems containing of one or more of the following building blocks: diffusion, convection, migration, reaction terms, network equations).

In this talk, we discuss progresses made for such PDE systems. The focus will be on approaches which have recently been or can easily be integrated into industrial simulation codes. In particular, we propose a new, automatic and adaptive solver and parameter switching strategy. Among important components are robust point-based AMG approaches with ILUT smoothing as well as an automatic ILUT-parameter switching strategy. We will present recent results for applications in industrial oil reservoir simulation and discuss promising extensions for other application classes.

High-performance parallel multigrid for large-scale shock physics simulations. **Jonathan Hu** (Sandia National Laboratories, USA) IC/MT3089/027

Parallel multigrid for large-scale shock physics simulations presents unique challenges, due to the need to simultaneously address parallel and algorithmic performance. System resources are often constrained because of demands from other parts of the application, coarse-level problems can have large communication to computation ratios, and load-balancing of the linear systems may be optimized for something other than the linear solver. We discuss our approaches to these challenges, and present numerical results on thousands of processors.

Smoothed agglomeration multigrid for incompressible flows. **Aleš Janka** (Université de Fribourg, Switzerland) IC/MT3164/027

We discuss advantages of using algebraic multigrid based on smoothed agglomeration for solving indefinite linear problems. The ingredients of smoothed agglomeration are used to construct a black-box monolithic multigrid method with idefinite coarse problems. Several techniques enforcing inf-sup stability conditions on coarse levels are presented. Numerical experiments are designed to support recent stability results for coupled algebraic multigrid. Comparison of the proposed multigrid preconditioner with other methods shows its robust behaviour even for very elongated geometries, where the pressure mass matrix is no longer a good preconditioner for the pressure Schur complement.

IC/MP239/027: Recent advances in algebraic multigrid with applications. #2

Organiser: Michael Gee (TU München, Germany)
Co-organiser: Marzio Sala (ETH Zürich, Switzerland)

(For abstract, see session #1 above.)

Long-range interpolation for parallel algebraic multigrid. **Ulrike Yang** (Lawrence Livermore National Laboratory, USA) IC/MT1323/027

Algebraic multigrid (AMG) is one of the most efficient and scalable parallel algorithms for solving sparse unstructured linear systems. However, for large three-dimensional problems, the coarse grids that are normally used in AMG often lead to growing complexity in terms of memory use and execution time per AMG V-cycle. Sparser coarse grids, such as the grids obtained by Parallel Modified Independent Set (PMIS) coarsening, compatible relaxation or aggressive coarsening remedy this complexity growth, but lead to non-scalable AMG convergence factors when traditional interpolation methods are used that include only distance-one coarse grid points in the interpolatory set. Since the coarse grid points are now located further apart and no longer meet criteria enforced in classical coarsening schemes, long range interpolation operators are needed.

In this paper we study the scalability of AMG methods that use sparser coarse grids, combined with long-range interpolation methods. AMG performance and scalability is compared for a variety of relevant test problems on parallel computers. It is shown that the increased interpolation accuracy largely restores the scalability of AMG convergence factors for PMIS-coarsened grids, without significantly affecting memory and execution time complexity per AMG V-cycle. This leads to a class of parallel AMG methods that enjoy excellent scalability properties on large parallel computers.

This is joint work with Hans De Sterck, Waterloo University, Josh Nolting, University of Colorado, and Rob Falgout, LLNL. This work was performed under the auspices of the U.S. Department of Energy by University of California Lawrence Livermore National Laboratory under contract number W-7405-Eng-48.

Maxwell's equations: discrete reformulation and algebraic multigrid solution. **Raymond Tuminaro** (Sandia National Laboratories, USA) IC/MT1584/027

We consider the linear solution of the eddy current equations. The large null space of the curl-curl operator within the eddy current equations complicates the application of most standard preconditioning techniques. Current solvers are often specialized techniques that cannot effectively leverage standard algebraic multigrid (AMG) methods and software for Laplace-type problems. We propose a new completely algebraic reformulation of the discrete eddy current equations along with a new AMG algorithm for this reformulated problem. The reformulation process takes advantage of a discrete Hodge decomposition to replace the discrete eddy current equations by an equivalent block 2x2 linear system whose diagonal blocks are discrete Hodge Laplace operators acting on edges and nodes, respectively. While this new AMG technique requires some special treatment in generating a grid transfer from the fine mesh, the coarser meshes can be handled using standard methods for Laplace-type problems. Our new AMG method is applicable to a wide range of compatible methods on structured and unstructured grids, including edge finite elements, mimetic finite differences, co-volume methods and Yee-like schemes. We illustrate the new technique, using edge elements in the context of smoothed aggregation AMG, and present computational results for problems in both two and three dimensions.

A multilevel method for discontinuous Galerkin finite-element equations: 3D anisotropic problems. **Johannes Kraus** (RICAM Linz, Austria), Satyendra Tomar (RICAM Linz, Austria) IC/MT3497/027

We construct optimal order multilevel preconditioners for certain discontinuous Galerkin (DG) finite element discretizations of three-dimensional (3D) anisotropic elliptic boundary-value problems. The presented approach has been introduced in an earlier work by the authors where the focus has been on 2D isotropic problems [1]. In this talk the analysis is extended, covering now 3D problems and incorporating the case of anisotropy. A specific assembling process is proposed which allows us to characterize the hierarchical splitting locally. This is also the key for a local analysis of the angle between the resulting subspaces. Applying the corresponding two-level basis transformation recursively, a sequence of algebraic problems is generated. It turns out that these discrete problems can be associated with coarse versions of DG approximations (of the solution to the original variational problem) on a hierarchy of geometrically nested meshes. New bounds for the constant γ in the strengthened Cauchy-Bunyakowski-Schwarz inequality are derived. The presented numerical results support the theoretical analysis and demonstrate the potential of this approach.

[1] J.K. Kraus and S.K.. Tomar: Multilevel preconditioning of elliptic problems discretized by a class of discontinuous Galerkin methods (submitted to SIAM J. Sci. Comput.)

A new smoothed aggregation multigrid method for anisotropic problems. **Michael Gee** (TU München, Germany), Raymond Tuminaro (Sandia National Laboratories, USA), Jonathan Hu (Sandia National Laboratories, USA) IC/MT2875/027

A new prolongator is proposed for smoothed aggregation multigrid. The proposed prolongator addresses a limitation of standard smoothed aggregation when it is applied to anisotropic problems. For anisotropic problems, it is fairly standard to generate small aggregates (used to mimic semi-coarsening) in order to only coarsen in directions of strong coupling. While beneficial to convergence, this can lead to a prohibitively large number of nonzeros in the standard smoothed aggregation prolongator and the corresponding coarse discretization operator. To avoid this, the new prolongator modifies the standard prolongator by shifting support (nonzeros within a prolongator column) from one aggregate to another to satisfy a specified nonzero pattern. This leads to a sparser operator which can be used effectively within a multigrid V-cycle. The key to this algorithm is that it preserves certain null space interpolation properties that are central to smoothed aggregation for both scalar and systems of PDEs. We present 2D and 3D numerical experiments that demonstrate that the new method is competitive with standard smoothed aggregation for scalar problems, and significantly better for problems arising from PDE systems.

IC/MP408/027: Adaptive and multilevel methods in electromagnetics.

Organiser: Ralf Hiptmair (ETH Zürich, Switzerland)
Co-organiser: Jinchao Xu (Pennsylvania State University, USA)

The finite-element or boundary-element discretization of quite a few variational problems arising in computational electromagnetics employs edge elements. As in other areas where finite elements are applied efficiency entails the use of fast multilevel iterative solvers and the adaptive choice of Galerkin trial spaces.

Talks in this minisymposium will provide a comprehensive survey of recent theoretical and algorithmic advances in the field of adaptive and multilevel methods in computational electromagnetics.

Local multigrids in electromagnetics. **Oliver Sterz** (Computer Simulation Technology, Germany) IC/MT1913/027

The efficient computation of electromagnetic problems requires adaptive methods in combination with fast iterative solvers like multigrid methods. In order to achieve potential optimality, standard implementations of multigrid schemes need a geometrical growth of the number of unknowns from one refinement level to the next. For adaptive computations this condition may be violated.

The concept of local multigrids can resolve the problem. This contribution provides an overview of the key aspects of an adaptive local multigrid scheme for electromagnetics including algorithmic details.

Local multigrid method in $H(\mathrm{curl})$. **Weiying Zheng** (Chinese Academy of Sciences), Ralf Hiptmair (ETH Zürich, Switzerland) IC/MT1341/027

We consider $\mathbf{H}(\mathbf{curl},\Omega)$-elliptic variational problems on bounded Lipschitz polyhedra and their finite element Galerkin discretization by means of lowest order edge elements. If the underlying mesh has been created by successive local mesh refinement, the so-called local multigrid correction scheme with hybrid smoothing provides a fast iterative solver for the resulting sparse linear system of equations. We review the convergence theory developed for local multigrid in a $H^1(\Omega)$-context and use it along with regular Helmholtz-type decompositions in order to establish asymptotic optimality of local multigrid for edge elements.

Auxiliary space preconditioners for electromagnetics. **Ralf Hiptmair** (ETH Zürich, Switzerland) IC/MT4840/027

We propose a general approach to preconditioning discrete $H(\mathbf{curl},\Omega)$-elliptic systems based on Poisson solvers. We prove mesh-independent effectiveness the preconditioners by appealing to the abstract theory of auxiliary space preconditioning. The main tool are discrete analogues of so-called regular decomposition results in the function space $H(\mathbf{curl},\Omega)$.

An important application of this general approach is the design of asymptotically efficient algebraic multigrid methods for the $H(\mathbf{curl})$-elliptic systems, based on algebraic multigrid methods for the discretized Poisson equation.

Parallel auxiliary space AMG for Maxwell problems. **Tzanio Kolev** (Lawrence Livermore National Laboratory, USA) IC/MT1317/027

Recently we implemented a parallel algebraic solver for definite Maxwell problems [1] based on the new Nedelec space decomposition by Hiptmair and Xu [2]. In this talk we are going to give an overview of the solver, and its numerical performance on large model electromagnetic problems. We will also consider several related methods, as well as extensions to more difficult problems.

[1] Tz. Kolev and P. Vassilevski, *Parallel H1-based auxiliary space AMG solver for H(curl) problems*, LLNL Technical Report 222763, 2006.

[2] R. Hiptmair and J. Xu, *Nodal Auxiliary Space Preconditioning in H(curl) and H(div) spaces*, ETH SAM Report 2006-09, 2006.

IC/MP408/027: Adaptive and multilevel methods in electromagnetics. #2

Organiser: Ralf Hiptmair (ETH Zürich, Switzerland)
Co-organiser: Jinchao Xu (Pennsylvania State University, USA)

(For abstract, see session #1 above.)

hp-adaptive finite-element methods for Maxwell's equations: an update. **Leszek Demkowicz** (University of Texas at Austin, USA) IC/MT4880/027

I will report on our current work directed at working out a fully-automatic hp-adaptive finite element methodology for solving 3D time-harmonic Maxwell equations. The presentation will include:

- a summary of a current theoretical work related to the subject, including a recent result on polynomial extensions for H^1, $H(\mathrm{curl})$, and $H(\mathrm{div})$-conforming spaces defined on a cube,
- a discussion of an implementation for PML and its use in 3D simulations,
- 3D numerical examples.

The results represent a joint work with many colleagues including J. Kurtz, M. Costabel and M. Dauge.

Uniform a posteriori *error estimation for the heterogeneous Maxwell equations.* **Serge Nicaise** (Université de Valenciennes, France) IC/MT3328/027

We consider different *a posteriori* error estimators for the heterogeneous Maxwell equations with discontinuous coefficients in a bounded two or three dimensional domains. The continuous problem is approximated using conforming approximated spaces. The main goal is to express the dependence of the constants in the lower and upper bounds with respect to chosen norm and to the variation of the coefficients. For that purpose, some new interpolants of Clément/Nédélec type are introduced and some interpolation error estimates are proved. Some appropriate Helmholtz decompositions are also requested. Some numerical tests will be presented which confirm our theoretical results.

Equilibrated residual-error estimators for Maxwell equations. **Joachim Schöberl** (RWTH Aachen, Germany) IC/MT3173/027

A posteriori error estimates without generic constants can be obtained by a comparison of the finite element solution with a feasible function for a dual problem. A cheap computation of such functions via equilibration is well-known for scalar equations of second order. We simplify and modify the equilibration such that it can be applied to Maxwell's equations and edge elements. The two key ingredients are exact sequences for distributional finite elements, and a divergence free local decomposition of the residual. Numerical results for eddy current problems are presented.

RICAM Report 2006-19 is available from http://www.ricam.oeaw.ac.at/publications

Convergence analysis of adaptive edge-element approximations of the 3D eddy-current equations. **Ronald Hoppe** (Universität Augsburg, Germany) IC/MT2882/027

We consider Adaptive Edge Finite Element Methods (AEFEM) for the 3D eddy currents equations with variable coefficients based on the lowest order edge elements of Nédélec's first family with respect to an adaptively generated hierarchy of simplicial triangulations. The mesh adaptivity relies on a residual-type a posteriori error estimator featuring face and element residuals. Both the components of the estimator and certain oscillation terms, due to the occurrence of the variable coefficients, have to be controlled properly within the adaptive loop which is taken care of by appropriate bulk criteria. Convergence of the AEFEM in terms of reductions of the energy norm of the discretization error and of the oscillations is shown. Numerical results are given to illustrate the performance of the AEFEM.

IC/MP166/027: Multigrid methods for systems of PDEs.

Organiser: Marcus Mohr (Universität München, Germany)
Co-organiser: Ulrich Rüde (Universität Erlangen-Nürnberg, Germany)

The last two decades have seen a steady increase in the interest in so called multigrid and mutilevel approaches for the solution of linear systems of equations arising from the discretisation of models described by partial differential equations. This phenomenon is primarily based on two factors. On the one hand side there is a constant growth in size and complexity of such models. On the other side optimally tuned multigrid methods can solve the associated linear systems with an amount of work that scales linearly with the number of unknowns. Making them especially interesting not only for stationary linear problems, but also for non-linear and time-dependent ones. Thus, multilevel methods have long transcended the realm of symmetric and positive definite problems for which they were originally designed.

However, in order to reach optimal convergence rates the individual components of a multilevel algorithm must always be adapted to the problem at hand. This can either be done manually for a concrete application or by automatic techniques as in blackbox and algebraic multigrid approaches. Systems of PDEs pose their very own challenges in this respect. Be it that many such applications are formulated as saddle point problems and the resulting indefinite linear algebraic problems require the classical point smoothers to be replaced by coupled or distributive relaxation approaches to reduce high-frequency error components. Be it that new methods are required in order to identify coarse error components and to construct coarse 'grids' in algebraic approaches for systems. Be it that schemes for the construction of operator dependent grid transfers in the case of strongly varying or jumping coefficients must be adapted from the scalar to the system setting.

This minisymposium aims at bringing together researchers from the multilevel community and from application areas where these methods are applied to systems of PDEs in order to present and discuss new concepts and ongoing research in this field. The talks will cover a broad range of applications and approaches ranging from geometric methods for systems resulting from the Finite Element discretisation of the generalised Stokes problem of geophysical mantle convection over multigrid methods applied to the poro-elasticity problem used for Finite Differences on staggered and collocated grids up to new approaches for systems in algebraic multigrid methods and problems in the new application area of image processing and optical flow.

Multigrid methods for the poroelasticity system. **Francisco Gaspar** (Universidad de Zaragoza, Spain), Lisbona Francisco (Universidad de Zaragoza, Spain), Cornelis Oosterlee (TU Delft, The Netherlands) IC/MT2972/027

In this talk, we present robust and efficient multigrid solvers for the poroelasticity system. We introduce a reformulation of the problem which enables us to treat the system in a decoupled fashion. This permits us to choose a highly efficient multigrid method for a scalar Poisson type equation for the overall solution of this poroelasticity system. With standard geometric transfer operators, a direct coarse grid discretization and a point-wise red-black Gauss-Seidel smoother, an efficient multigrid method is developed for all relevant choices of the problem parameters. The transformation boils down to a stabilization term in the original formulation for which a highly efficient multigrid solver also can be developed. A relation between the multigrid treatment of poro-elasticity and the Stokes equations is also included in this talk.

Generation of coarse-grid approximations for systems of PDEs with discontinuous coefficients. **Marcus Mohr** (Universität München, Germany), Harald Köstler (Universität Erlangen–Nürnberg, Germany), Ulrich Rüde (Universität Erlangen–Nürnberg, Germany) IC/MT1414/027

Multigrid methods are well-known for combining fast convergence speeds with low costs per individual iteration step when applied for the solution of linear systems arising from elliptic partial differential equations (PDEs). However, in order to reach the ultimate goal of linear $\mathcal{O}(n)$ efficiency for solving such problems the interplay of the individual components that make up a multigrid method must be optimal. In detail these components are smoother, grid coarsening strategy, inter-grid transfer operators and the coarse grid approximation of the fine grid operator.

This talk considers the construction of the latter component for the special situation that the linear system under consideration stems from the discretisation of a system of PDEs and features strongly varying or discontinuous coefficients. This situation arises in many practical applications, e.g. optical flow reconstruction in image processing or simulation of mantle convection in geophysics. We report on different approaches that extend the classical techniques for the case of scalar-valued stencil coefficients to the case of tensor-valued entries and present examples from the two application fields mentioned above.

Coarse-grid selection for systems of PDEs based on compatible relaxation. **Robert Falgout** (Lawrence Livermore National Laboratory, USA) IC/MT2581/027

Algebraic multigrid is an important method for solving the large sparse linear systems that arise in many PDE-based scientific simulation codes. A major component of algebraic multigrid methods is the selection of coarse grids.

The notion of *compatible relaxation* (CR) was introduced by Brandt in [1] as a modified relaxation scheme that keeps the coarse-level variables invariant. Brandt states that the convergence rate of CR is a general measure for the quality of the set of coarse variables, and in [2], we developed a supporting theory for this idea. We have since developed an algebraic coarsening algorithm based on compatible relaxation that has several nice properties over the classical coarsening schemes. One such characteristic is its ability to ensure the quality of the coarse grid. However, our original method has the potential to overselect coarse-grid points when applied to PDE systems problems.

In this talk, we will describe recent progress developing a systems version of our coarsening algorithm, point out its current strengths and weaknesses, and discuss open questions and future directions.

This work was performed under the auspices of the U.S. Department of Energy by University of California Lawrence Livermore National Laboratory under contract No. W-7405-Eng-48.

[1] A. Brandt, *General highly accurate algebraic coarsening*, Electronic Transactions on Numerical Analysis, 10 (2000), pp. 1–20.

[2] R. D. Falgout and P. S. Vassilevski, *On generalizing the AMG framework*, SIAM J. Numer. Anal., 42 (2004), pp. 1669–1693. UCRL-JC-150807.

IC/MP650/027: Adaptive and multilevel methods: design, analysis, and application.

Organiser: Ricardo Nochetto (University of Maryland, USA)
Co-organiser: Jinchao Xu (Pennsylvania State University, USA)
Co-organiser: Kunibert Siebert (Universität Augsburg, Germany)

This minisymposium will explore a more complete integration of adaptive and multilevel algorithms, in terms of algorithm design, convergence and complexity theory, and application to important problems in science and engineering. This endeavor is expected to foster the theoretical foundations for the combined use of modern techniques in adaptivity and multilevel solvers, leading to general principles and guidelines for designing and applying adaptive and multilevel algorithms in an integrated fashion, with the goal of improving the effectiveness of mult-ilevel adaptive methods in various applications. This combination of theoretical and algorithmic design framework will be positioned to have substantial impact in the multiscale/multiphysics modeling areas, which draw on ideas from both the multilevel and adaptivity areas independently. Since applications truly drive the research in multiscale modeling, the list of tentative speakers reflects our intent of mixing basic research with applications as well as numerical techniques such as adaptive finite elements methods (AFEM) with wavelets.

A list of fundamental challenges to be discussed in the minisymposium follows:

- Convergence and optimality of AFEM for general elliptic operators.
- Multigrid methods for PDE with discontinuous and degenerate coefficients. Anisotropic refinement/coarsening.
- Algebraic multigrid for AFEM: design and convergence analysis.
- Parallel AFEM: design, convergence, and optimality.
- AFEM and wavelets for nonlinear PDE.
- AFEM for geometric flows: design and analysis.
- Multilevel AFEM for porous media and complex fluids.

A basic convergence result for conforming adaptive finite elements. **Andreas Veeser** (Università degli Studi di Milano, Italy), Pedro Morin (Universidad Nacional del Litoral, Argentina), Kunibert Siebert (Universität Augsburg, Germany) IC/MT2739/027

We consider the approximate solution with adaptive finite elements of a class of linear boundary value problems, which includes problems of 'saddle point' type. Supposing that refinement relies on unique quasi-regular element subdivisions and leads to locally quasi-uniform grids, that the finite element spaces are conforming, nested, and satisfy the inf-sup conditions, that the error estimator is reliable as well as locally and discretely efficient, and that marked elements are subdivided at least once, we give a sufficient and essentially necessary condition on marking for the convergence of the finite element solutions to the exact one. This condition is not only satisfied by Dörfler's strategy, but also by the maximum strategy and the equidistribution strategy.

An optimal adaptive finite-element method. **Rob Stevenson** (Universiteit Utrecht, The Netherlands) IC/MT2373/027

We present a construction an adaptive finite element method for solving elliptic equations in d space dimensions that has optimal computational complexity. Whenever for some $s > 0$, the solution can be approximated to accuracy $\mathcal{O}(N^{-s})$ in energy norm by a continuous piecewise polynomial of degree k on some partition into N d-simplices, and one knows how to approximate the right-hand side in the dual norm with the same rate with piecewise polynomials of degree $k-1$, then the adaptive method produces approximations that converge with this rate, taking a number of operations that is of the order of the number of simplices in the output partition. The method is similar in spirit to that from [*SINUM*, 38 (2000), pp.466–488] by Morin, Nochetto, and Siebert, and so in particular it does not rely on a recurrent coarsening of the partitions.

When time allows, as extensions we discuss a new optimal goal oriented adaptive finite element method, and such a method for solving the Stokes equations, and illustrate our findings with numerical results.

Convergence and optimality of AFEM for general second-order linear elliptic operators. **Ricardo Nochetto** (University of Maryland, USA), Kunibert Siebert (Universität Augsburg, Germany) IC/MT3799/027

We analyze the simplest and most standard adaptive finite element method (AFEM), with any polynomial degree, for general second order linear, symmetric elliptic operators. As it is customary in practice, AFEM marks exclusively according to the error estimator and performs a minimal element refinement without the interior node property. We prove that AFEM is a contraction for the sum of energy error and scaled error estimator, between two consecutive adaptive loops. This geometric decay is instrumental to derive optimal cardinality of AFEM. We show that AFEM yields a decay rate of energy error plus oscillation in terms of number of degrees of freedom as dictated by the best approximation for this combined nonlinear quantity. This is joint work with J.M. Cascon, C. Kreuzer, and K.G. Siebert.

A new class of anisotropic smoothness spaces. **Ronald DeVore** (University of South Carolina, USA) IC/MT3740/027

We introducee a new class of smoothness spaces based on the level sets of a function. These spaces can already be shown to effectively describe images which can be well compressed. They could potentially be useful in constructing and analyzing adaptive methods for nonlinear evolution equations because of their anisotropic character. We will describe these spaces and some of their properties.

IC/MP650/027: Adaptive and multilevel methods: design, analysis, and application. #2

Organiser: Ricardo Nochetto (University of Maryland, USA)
Co-organiser: Jinchao Xu (Pennsylvania State University, USA)
Co-organiser: Kunibert Siebert (Universität Augsburg, Germany)

(For abstract, see session #1 above.)

Regular decompositions and multigrid analysis. **Ralf Hiptmair** (ETH Zürich, Switzerland) IC/MT3735/027

Regular decompositions provide stable splittings of Sobolev spaces of div- and curl-conforming vector fields into an H^1-regular component and a contribution from the kernel of the differential operator. It has turned out that these decompositions hold the key to regularity-free multigrid theory for discrete $\mathbf{H}(\mathrm{curl},\Omega)$- and $\mathbf{H}(\mathrm{div},\Omega)$-elliptic variational problems. They have also inspired the construction of new auxiliary space methods. The talk will give a survey of regular decompositions and explain how they pave the way for harnessing the power of multilevel theory in H^1 for vector-valued variational problems.

Hierarchical error estimates for contact problems. **Ralf Kornhuber** (Freie Universität Berlin, Germany), Oliver Sander (Freie Universität Berlin, Germany) IC/MT3804/027

Hierarchical error estimates are based on the solution of local subproblems associated with an enlarged trial space. In the linear self-adjoint case, the resulting error indicators are locally equivalent to well-known residual-based estimates. In this talk, we discuss recent extensions to contact problems in continuum mechanics.

Error reduction in adaptive finite-element methods for elliptic obstacle problems. **Ronald Hoppe** (Universität Augsburg, Germany) IC/MT2889/027

An *a posteriori* error analysis for finite element approximations of elliptic obstacle problems on the basis of residual and hierarchical type *a posteriori* error estimators has been provided in a series of papers. In this contribution, we are concerned with a convergence analysis of adaptive finite element methods. We are using a residual error estimator which is a slight modification of that known from the unconstrained case. The ingredients of the convergence analysis are the reliability of the estimator, its discrete local efficiency, and an appropriate bulk criterion for the refinement process. Numerical results are given to illustrate the performance of the estimator.

Convergent adaptive approximation of some nonlinear elliptic problems. **Michael Holst** (University of California, San Diego, USA) IC/MT3424/027

We examine two nonlinear PDE models arising in biophysics and geometric analysis. We begin by establishing basic results and max-norm estimates. We then derive *a priori* and *a posteriori* estimates for Galerkin approximations, and describe a nonlinear approximation algorithm based on error indicator-driven adaptive refinement. We then develop some convergence results for the adaptive algorithm applied to each nonlinear problems. We finish by illustrating the adaptive algorithm with examples using the Finite Element ToolKit (FETK).

Portions of this work are joint with Long Chen and Jinchao Xu.

IC/MP139/015: Recent advances in numerical multiscale methods.

Organiser: Giovanni Samaey (Katholieke Universiteit Leuven, Belgium)
Co-organiser: Dirk Roose (Katholieke Universiteit Leuven, Belgium)

For many problems, ranging from hydrodynamics to chemistry and mathematical biology, one can only model the system dynamics with sufficient accuracy by including effects on microscopic scales. Due to the computational complexity, direct simulation using standard numerical methods then quickly becomes prohibitively expensive. However, we are often only interested in the system dynamics on macroscopic scales.

Therefore, there is an active interest in developing *multiscale* numerical algorithms, which aim at bridging the gap between the (microscopic) scale at which a model is given, and the (macroscopic) scale at which we would like to observe and analyse the system. This minisymposium provides an overview of some recently developed methods.

The first session is devoted to the class of so-called *equation-free* methods, as proposed by Kevrekidis *et al.* This framework assumes that a closed model *exists* (conceptually) for an appropriate set of macroscopic observables, which cannot be derived explicitly from the underlying microscopic model without making simplifications that are hard to justify. The main idea is to design *computational experiments* with the microscopic model to estimate macroscopic time derivatives; these experiments replace function evaluations which would normally have been obtained using the macroscopic model. The speakers will discuss issues of initialization, accuracy and efficiency and show a number of applications.

The second session addresses numerical methods for multiscale partial differential equations. Due to small-scale heterogeneities, the system parameters often exhibit randomness; the aim is to obtain appropriate statistics of the behaviour on macroscopic scales. The speakers will discuss numerical upscaling techniques to obtain homogenised coefficients, uncertainty quantification, patch dynamics and algorithm refinement methods.

From microscopic to macroscopic behaviour in biological systems. **Radek Erban** (University of Oxford, UK) IC/MT688/0

We present analytical (derivation of macroscopic equations) and computational (macroscopic equation-free) approaches for extracting a population-level behaviour from individual-based models of biological systems. We consider systems of many individuals (molecules, cells, organisms) for which the stochastic individual-based (microscopic) models are given and we study their macroscopic (collective, coarse-grained) behaviour. The biological examples include dispersal of unicellular organisms (e.g. bacterium Escherichia coli or amoeboid cell Dictyostelium discoideum) and models of gene regulatory networks.

Analysis of the constrained-runs reduction scheme. **Antonios Zagaris** (CWI, Amsterdam, The Netherlands) IC/MT1865/0

Microscopic and detailed macroscopic modelling often leads to large systems whose dynamics occur in a broad range of time scales. Multiscale reduction methods exploit the time-scale disparity present in a system to derive a simplified description of it, which is valid after the short initial transients have relaxed and captures the eventual dynamics. In this way, numerical stiffness may be removed and simulation times radically decreased, thus paving the way to the efficient modelling of many complex systems.

Recently, a family of reduction methods was proposed with the scope of assisting efficient, equation-free implementations of the projective integration schemes developed by C.W. Gear and I.G. Kevrekidis. These methods have also found application in hybrid modelling—in particular, in matching the state variables used in different spatial regions across the interface smoothly. In this talk, I will identify the principle underlying these methods and examine its accuracy in the context of singularly-perturbed dynamical systems. Further, I will consider simple computational realizations of these methods and examine analytically their stability properties. I will conclude with a short discussion of possible stabilization schemes and other future extensions of this work.

This is joint work with: C.W. Gear, I.G. Kevrekidis, and T.J. Kaper.

Numerical analysis of the accelerated coarse time-stepper for a lattice-Boltzmann model. **Christophe Vandekerckhove** (Katholieke Universiteit Leuven, Belgium), Dirk Roose (Katholieke Universiteit Leuven, Belgium) IC/MT3168/0

In current modelling practice, the best available model is often given on a microscopic level, while one is only interested in the coarser, macroscopic behaviour of the system. For this class of problems, Kevrekidis and coworkers have developed the equation-free computing approach, which uses appropriately initialized microscopic simulations to perform traditional macroscopic tasks, hereby circumventing the theoretical derivation of macroscopic evolution equations.

The basic tool is the so-called coarse time-stepper. An essential component is the lifting step in which a macroscopic field is mapped to the higher-dimensional space of microscopic variables. As this lifting step is not unique, it is often non-trivial to implement. In this context, the constrained runs algorithm was proposed to compute an appropriate microscopic state. The purpose of this talk is to study several aspects of the equation-free approach for a lattice Boltzmann model of a reaction-diffusion system. We first show how the lifting influences the accuracy and the stability of the resulting coarse time-stepper. Then, we show that, depending on the model parameters, the constrained runs iteration may converge very slowly or that it may even diverge. An alternative implementation based on a preconditioned Newton-Krylov method is therefore presented and tested for the lattice Boltzmann model. Finally, we demonstrate that once an appropriate coarse time-stepper is constructed, it can be accelerated substantially using the recently proposed teleprojective integrators or the multistep state extrapolation method.

Coarse-grained computations for agent-based models. **Yannis Kevrekidis** (Princeton University, USA) IC/MT3034/0

We will discuss recent advances in equation-free computation of fine-scale models. In particular, we will study how equation-free methods can be linked to data mining algorithms for the on-line "discovery" of good coarse-grained observables.

IC/MP139/015: Recent advances in numerical multiscale methods. #2

Organiser: Giovanni Samaey (Katholieke Universiteit Leuven, Belgium)
Co-organiser: Dirk Roose (Katholieke Universiteit Leuven, Belgium)

(For abstract, see session #1 above.)

Patch dynamics: macroscopic simulation of multiscale systems. **Giovanni Samaey** (Katholieke Universiteit Leuven, Belgium), Yannis Kevrekidis (Princeton University, USA), Dirk Roose (Katholieke Universiteit Leuven, Belgium) IC/MT1822/0

For an important class of multiscale problems, a separation of scales exists between the available (microscopic) model and the (macroscopic) level at which one would like to observe and analyze the system. For time-dependent multiscale problems of this type, Kevrekidis et al. developed a so-called "equation-free" framework, based on the idea of a so-called coarse-grained time-stepper. The patch dynamics scheme is a coarse-grained time-stepper which approximates the time evolution of a set of spatially distributed macroscopic variables for which the governing partial differential equation (PDE) is not (or only approximately) available; the scheme only performs appropriately initialized simulations using the available microscopic model in small portions of the space-time domain (the patches).

We present some theoretical and numerical convergence results for a class of parabolic homogenization problems. In particular, we show that the scheme approximates a finite difference scheme for the unavailable macroscopic equation. We also formulate and analyze a finite volume variant, and discuss some issues that arise when trying to combine patch dynamics with adaptive mesh refinement (AMR). We conclude with a brief discussion of the possibilities and limitations of the current schemes, and provide some ideas for future research.

Modeling of fluctuations in algorithm refinement methods. **John Bell** (Lawrence Berkeley National Laboratory, USA) IC/MT1480/0

We consider an approach for hybrid algorithms based on an adaptive mesh refinement paradigm. In this approach a hierarchical adaptive mesh refinement framework is used to embed a particle algorithm within the finest grid of the mesh hierarchy. The coupling between the particle region and the overlaying continuum grid is functionally equivalent to that between fine and coarse levels of mesh refinement. In this paper we consider the role of fluctuations in this type of hybrid algorithm. In particular, we discuss the impact of fluctuations on the dynamics. We demonstrate that it is necessary to include a stochastic forcing term to model fluctuations at the continuum level to accurately capture the correct behavior of the system. We illustrate the role of fluctuations on two model problems. In the first we consider an excluded random walk model whose mean field behavior is given by the viscous Burgers' equation. The second example discusses a hybrid of direct simulation Monte Carlo with the compressible Navier Stokes equations. For the Navier Stokes equations we include stochastic fluxes as given by Landau-Lifshitz fluctuation Navier-Stokes equations.

Equation-free methods for molecular dynamics: a lifting procedure. **Yves Frederix** (Katholieke Universiteit Leuven, Belgium), Dirk Roose (Katholieke Universiteit Leuven, Belgium) IC/MT5043/0

The equation-free framework as proposed by Kevrekidis *et al.* offers a methodology to compute the macroscopic system dynamics using only a description on the microscopic level. This technique is especially suitable when the macroscopic equations are unknown or cannot be derived in a closed form. Short bursts of the microscopic simulation code are combined with appropriate lifting (initialization) and restriction (averaging) operators to cross the boundaries between micro- and macroscopic scale. The resulting time integrator defines the so-called coarse time stepper and enables the microscopic code to perform system-level tasks.

In this work we use molecular dynamics as the microscopic simulator and investigate the difficulties that can arise when using this type of microscopic description. An important issue is the appropriate initialization of the microscopic simulator in order to obtain the correct coarse dynamics. We will define good lifting and restriction operators, based on kernel density estimation, which are suited for use in the equation-free framework. We present a model problem where we aim at calculating a coarse steady state of a time evolving probability density function, and use it as an illustration for the proposed operators.

IC/MP695/027: *A posteriori* error estimates and multi-grid methods for eigenvalue problems.

Organiser: Ludmil Zikatanov (Pennsylvania State University, USA)
Co-organiser: Daniele Boffi (Università degli Studi di Pavia, Italy)

The main theme of the minisymposium is on the advanced finite element and multigrid techniques for eigenvalue problems. The focus is on the *a posteriori* error estimation and the design of adaptive tools both at the discretization stage and for the solution of the resulting large-scale linear and nonlinear discrete problems. Examples of potential applications of these techniques are found in numerical models used in electromagnetics, flow simulation, elasticity and quantum chromodynamics and other.

Towards adaptive multigrid eigenvalue computation. **Carsten Carstensen** (Department of Mathematics Humboldt-Universität, Germany), Ira Livshits (Ball State University, USA) IC/MT3640/027

The presentation concerns the effective and reliable computation of PDE eigenvalue computation of model problems with adaptive mesh-refining algorithms and fast multigrid solvers. The reliable *a posteriori* error control of some finite element discretisation is reviewed from the literature. The approaches by Rannacher et al. and Larsson et al. are compared and some illustrative adaptive finite element cacluations will be presented. Multigrid methods have shown to be efficient for solving a variety of eigenvalue problems by exploiting different smoothness properties of operators and solutions. They are also benefitial for fast and accurate evaluation of global properties: such as eigenvalues, and this makes them even more attractive for the task. In this talk we discuss the current developments in the field of multigrid solvers for eigen problems, including an idea of multiscale eigenbasis that allows fast approximation of many eigenfunctions at once.

Multigrid/multiscale approach for finding a full eigen-basis of differential operators. **Ira Livshits** (Ball State University, USA) IC/MT4910/027

In this talk we will discuss how to apply multigrid methods to the discretized differential eigenvalue problems if the goal is to find not one but rather all eigenfunctions and eigenvalues of the finest discrete operators. The challenge here is to allow representation of all such eigenfunctions on the increasingly coarser grids, and do it accurately. The proposed solver uses the Multigrid Eigenbasis (MEB) structure for eigenfunction representation and employees special types of prolongation and restriction operators. The strategies of choosing such operators will be discussed on different examples, in particular, the Schrodinger eigenvalue problem. Numerical experiments and discussion of possible extensions of presented results conclude the talk. (Joint work with Achi Brandt.)

Mixed approximation of eigenvalue problems: a super-convergence result. **Daniele Boffi** (Università degli Studi di Pavia, Italy), Francesca Gardini (Università di Pavia, Italy) IC/MT3981/027

In this talk we present a superconvergence result for the lowest-order Raviart-Thomas approximation of eigenvalue problems. It is well-known that a similar superconvergence property holds for the mixed approximation of Laplace problem.

Here we introduce a new proof, since the one given for the source problem cannot be generalized in a straightforward way to the eigenvalue problem. Indeed, the key point of the proof strongly relies on the Galerkin orthogonality, which holds for the source problem but not for the eigenvalue one.

In order to prove the superconvergence property we will use the equivalence between the lowest order Raviart-Thomas approximation of Laplace eigenproblem with Neumann boundary conditions and the non-conforming piecewise linear Crouziex-Raviart approximation. We will also make use of a superconvergence result proved by Duran et al. for Laplace eigenproblem with Dirichlet boundary conditions.

Using this result, we introduce a reliable and efficient *a posteriori* error estimator for the lowest order Raviart-Thomas approximation of Laplace eigenproblem.

Eventually, we will show some numerical experiment which confirm the superconvergence property and suggest that it also holds for the lowest order Brezzi-Douglas-Marini approximation.

An adaptive multigrid method for the Dirac equations in lattice QCD. **James Brannick** (Pennsylvania State University, USA) IC/MT4004/027

Classical multigrid (MG) methods assume explicit knowledge of so-called algebraically-smooth or near-kernel components, which loosely speaking are errors that give relatively small residuals. Tyically, these methods generate a sequence of coarse spaces under the assumption that the near-kernel is locally constant. The difficulty in applying MG to discretizations of Quantum Chromodynamics (QCD) on a lattice is that the near-kernel components of the resulting Dirac matrix can be far from constant, often exhibiting little or no apparent smoothness. In fact, the local character of these components is random, depending on the randomness of the gluon fields. As a result, no apriori knowledge of the local character of the near-kernel of the Dirac operator is readily available.

In this talk we present a recently developed complex-arithmetic adaptive MG preconditioner suitable for the linear systems arising in lattice QCD. The method is an extension of the adaptive smoothed aggregation iterative solver in which good convergence properties are achieved in situations where explicit knowledge of the near-kernel components are not available. This extension is accomplished using the method itself to define a multilevel power iteration to expose the near-kernel. The coarsening process is then modified to both use and improve these computed components. Numerical results are presented to demonstrate the efficacy of the method.

IC/MP527/028: From differential geometry to compatible discretization.

Organiser: Ralf Hiptmair (ETH Zürich, Switzerland)
Co-organiser: Douglas Arnold (University of Minnesota, USA)

Recent years have seen tremendous progress in the transfer of ideas and concept from differential geometry to the discrete realm. Yet, we are only at the beginning of a development that has had and will have a powerful impact in areas as diverse as numerical methods for ordinary and partial differential equations and computer graphics.

This minisymposium aims to bring together leading researchers who have worked on various aspects of discrete differential geometry and related compatible discretizations. Their presentations will provide a survey of this exciting development, illuminating it from different perspectives and from different areas of application.

Discrete calculus of chainlet theory. **Jenny Harrison** (University of California, Berkeley, USA) IC/MT3972/028

This talk concerns the "missing half" of calculus – the study of k-dimensional domains of integration in n-space called "chainlets" matching the classical calculus of functions and forms. The chainlet operators, products and integrals apply to both symmetric and antisymmetric tensors yielding the full calculus on Euclidean space, cell complexes, manifolds with corners and cusps, bilayer structures (e.g., soap films), and nonsmooth domains such as fractals with equal ease. The resulting theory unifies and extends several classical viewpoints, from the discrete simplicial complex to the continuum theory of the exterior calculus. As time permits, we shall discuss applications to differential geometry and particle physics.

Discrete mechanics, DEC and optimization. **Jerrold Marsden** (California Institute of Technology, USA) IC/MT4807/028

This talk will present some work on discrete mechanics, differential exterior calculus and optimization. The DEC work concerns electromagnetism, the Yee scheme and its generalization to nonregular meshes, following Bossavit and others. The optimization work concerns the use of discrete mechanics together with SQP methods to solve optimization problems in robotics and satellite reorientation, for example.

Joint work with Mathieu Desbrun, Ari Stern, Sigrid Leyendecker and others.

Smoothed projections in finite-element exterior calculus. **Ragnar Winther** (Universitetet i Oslo, Norway) IC/MT2629/028

A classical problem in the analysis of mixed finite element methods is that the canonical interpolation operators onto the finite element spaces are not bounded with respect to the natural Sobolev norm. As a consequence, additional properties like extra regularity have to be introduced to establish stability. In this talk we will discuss how this problem can be avoided by constructing so-called smoothed projections, and how the properties of these operators lead directly to various stability properties of the corresponding discretizations of the Hodge-Laplace problem.

Smooth bases for discrete exterior calculus through subdivision. **Peter Schröder** (California Institute of Technology, USA) IC/MT4846/028

The basic approach to discrete exterior calculus on simplicial meshes in effect amounts to the use of certain linear finite elements (Whitney elements) when seen from a FEM point of view. A natural question then is whether one can exhibit smoother bases. One avenue is local enrichment with higher order polynomials. This leads to constructions in which multiple degrees of freedom *live* at simplicies of several dimensions for each of the underlying form fields. Instead we chose to go a different route. Fixing the simplicial co-boundary operator as the discrete d and demanding that there continue to be only single degrees of freedom per simplex, we produce smoother bases (with somewhat larger support) through subdivision. The resulting bases can be seen as generalizations of certain spline constructions. Since they are refinable they also come with attractive multigrid properties. In my presentation I will give a brief introduction to subdivision; i.e., the construction of

smooth functions (forms) through refinement and then discuss the central idea in our construction: ensuring that the subdivision operators commute with the discrete d.

IC/MP527/028: From differential geometry to compatible discretization. #2

Organiser: Ralf Hiptmair (ETH Zürich, Switzerland)
Co-organiser: Douglas Arnold (University of Minnesota, USA)

(For abstract, see session #1 above.)

Knotted linear force-free magnetic fields: topological aspects. **P. Robert Kotiuga** (Boston University, USA) IC/MT3592/028

Force-free magnetic fields, that is current distributions with vanishing Lorentz force, can be constructed from the eigenfunctions of the curl operator. A key obstacle is that when vector fields are restricted to be solenoidal, and the region of interest is restricted to be a compact manifold with boundary, the boundary conditions which render the curl and curl-curl operators self-adjoint, are mutually exclusive. Therefore, one cannot directly exploit the experience gained in electromagnetic cavity resonator calculations in the eigenvalue problem for the curl operator. Early calculations of linear force-free magnetic fields considered unbounded domains and sidestepped this problem by doing so. Later authors considered simply connected regions or unknotted multiply-connected regions. In more recent work a general study of self-adjoint curl operators is undertaken within a framework which accounts for knotted domains associated with the conjectured topological characteristics of force-free mgnetic fields. A caveat in finding boundary conditions which render the curl operator self-adjoint on a compact multiply-connected domain, is that the they are neccessarily nonlocal. Fortunately, the nonlocality can be articulated in terms of a symplectic form on the first homology group of the boundary, and handled systematically.

In this presentation, we formulate the b.v.p., emphasize the role of isotopy-invariant boundary conditions on multiply connected domains, and introduce notions from low-dimensional topology, such as the Torelli group, which articulate the difference between intuitive but noncomputable, versus formal but computable, aspects of formulating a well-posed b.v.p. on knotted domains.

Bibliography: Hiptmair, R., Kotiuga, P.R., Tordeux, S., "Selfadjoint curl operators," in preparation.

Geometric discretisation of Einstein's equations. **Jörg Frauendiener** (Universitetet i Oslo, Germany) IC/MT4841/028

Einstein's theory of gravity is a geometric theory. It describes a gravitating system as a Ricci-flat Lorentzian manifold. As such it is invariant under diffeomorphisms which implies that individual points have no physical meaning. Only relations between several points are physically and geometrically meaningful. In this talk I present an approach to computational GR which is based on a discrete formulation of a geometry i.e., on quantities defined on higher dimensional structures. We show that one can reproduce exact spherically symmetric solutions of Einstein's equations and plane waves.

Application of finite-element exterior calculus to elasticity. **Richard Falk** (Rutgers University, USA) IC/MT4842/028

It is now understood that there is a close connection between finite element differential complexes and the stability of finite element methods for the approximation of a wide variety of systems of partial differential equations. By exploiting a connection between a differential complex related to the equations of elasticity and the de Rham complex, we show how a new simple class of stable finite element approximations for the equations of elasticity can be developed.

Compatible discretization for the Helmholtz equation. **Joachim Schöberl** (RWTH Aachen, Germany) IC/MT3174/028

This talk addresses the finite element discretization of resonance problems. The PML method is applied to truncate the originally unbounded domain at a finite radius. As it is well know, the PML method introduces artificial eigenvalues which depend on the PML parameter. Additional spurious eigenvalues are introduced by a conforming finite element discretization. In contrast to the PML eigenvalues, these FEM eigenvalues are not well separated from the physical ones. By mesh refinement, or by increasing the polynomial order of the finite elements, the spurious eigenvalues near the real axis can be reduced. This is a quantitative improvement.

In this talk we present a finite element method which avoids the spurious FEM eigenvalues. In the one dimensional case, the modified method can be implemented by an integration formula of reduced order. We propose a mixed method which can be applied also for the two and three dimensional case. We will present numerical examples, and the current, not yet complete state of the analysis.

IC/MP357/015: Numerical methods for data-assimilation problems.

Organiser: Angelika Bunse-Gerstner (Universität Bremen, Germany)
Co-organiser: Nancy Nichols (University of Reading, UK)

For the very large systems that arise in the environmental sciences, the available data are not sufficient to initiate a complex computational forecasting model. The technique of data assimilation enables measured observations (over time) to be combined with model predictions to generate accurate estimates of the system states, both current and future. The problem of data assimilation is essentially an ill-posed inverse problem. An overview of data assimilation will be presented here and the major types of assimilation method for treating very large nonlinear systems will be described. New numerical techniques for improving the computational efficiency of these procedures will be presented and some practical applications from atmosphere and ocean modelling will be discussed.

Overview of data assimilation and the application of model reduction for optimal-state estimation in very-large systems. **Nancy Nichols** (University of Reading, UK) IC/MT3838/015

The problem of data assimilation can be treated either by sequential techniques based on optimal filtering methods, or by variational techniques that aim to solve an optimization problem subject to a set of dynamical system equations. For the very large inverse problems arising in the prediction of atmosphere and ocean circulations and other environmental systems, these methods are too costly to be used for real-time forecasting, and approximations are needed for computational efficiency. In this talk, we will give a brief overview of the data assimilation methods currently applied in practice and describe some current research issues. Model reduction techniques from control theory provide an attractive method for improving the computational efficiency of data assimilation schemes. Recently we have investigated the use of reduced order models with Gauss-Newton iteration for solving four-dimensional variational data assimilation problems. Results obtained using a balanced-truncation model reduction method in a simple shallow water test case are presented. The results illustrate the superior performance of this approach and show that the same accuracy in the solution can be obtained more efficiently by model reduction than by the standard procedures.

For the very large unstable models arising in environmental systems, however, the balanced-truncation method is not suitable and new techniques are needed to enable this approach to be applied. In the subsequent papers in this mini-symposium, this issue and other new assimilation techniques are discussed. *This work is joint with A.S. Lawless of the University of Reading, UK, and C. Boess and A. Bunse-Gerstner of the University of Bremen, Germany.

Interpolation-based model reduction for data assimilation. **Angelika Bunse-Gerstner** (Universität Bremen, Germany) IC/MT3851/015

The first talk in this mini-symposium shows that model reduction methods can in fact improve the computational efficiency of data assimilation schemes. They decrease the computational complexity considerably by generating reduced order linear dynamical systems which behave similar to the linearisations of the model for the environmental systems used within the Gauss–Newton iteration steps. To make this approach feasible for realistic problems we need model reduction methods which can handle the very large dimensions of the original very large dynamical systems. Numerical methods based on rational interpolation via Krylov space projections are attractive for these very large dimensions. There one would like to choose the interpolation points such that the behaviour of the reduced system is a reasonable overall approximation to the corresponding original system. In this talk we give a brief survey on rational interpolation methods as well as their generalization to tangential interpolation to point out the computations needed for these interpolation based reductions. Necessary conditions for so-called H_2-optimal model reduction are shown, from which we derive a good choice of interpolation points to get reasonable approximations.

This work is joint with Dorota Kubalinska of the University of Bremen, Germany.

Unbiased square-root ensemble filters for high-impact weather prediction. **Sarah Dance** (University of Reading, UK) IC/MT562/015

Numerical weather prediction models require an estimate of the current state of the atmosphere as an initial condition. Observations only provide partial information, so they are usually combined with prior information, in a process called data assimilation. The dynamics of hazardous weather such as storms is very nonlinear, with only a short predictability timescale, thus it is important to use a nonlinear, probabilistic filtering method to provide the initial conditions. Unfortunately, the state space is very large (about 10^7 variables) so approximations have to be made. The ensemble square root filter is a quasi-linear filter that has recently been proposed in the meteorological and oceanographic literature to solve this problem. The filter uses a forecast ensemble (a Monte Carlo sample) to estimate the prior statistics. In this talk we will describe the ensemble filter framework and some of its strengths and weaknesses. In particular we will demonstrate a new result that not all filters of this type bear the desired relationship to the forecast ensemble: there can be a systematic bias in the analysis ensemble mean and consequently an accompanying shortfall in the spread of the analysis ensemble as expressed by the ensemble covariance matrix. This points to the need for a restricted version of the notion of an ensemble square root filter. We have established a set of necessary and sufficient conditions for the scheme to be unbiased. Whilst these conditions are not a cure-all and cannot deal with independent sources of bias such as modelling errors, they should be useful to designers of ensmeble filters in the future. Work done in collaboration with Nancy Nichols and David Livings at the University of Reading. Work supported in part by the NERC National Centre for Atmospheric Sciences, an RCUK Academic Fellowship and by the NERC Data Assimilation Research Centre.

Variational assimilation of Lagrangian data in oceanography. **Maëlle Nodet** (Université Grenoble I, France) IC/MT3841/015

Within the framework of Global Ocean Data Assimilation Experiment (GODAE), an increasing amount of data are available. A crucial issue for oceanographers is to exploit at best these observations, in order to improve models, climatology, forecasts, etc. Thanks to the international program Argo and to more localized experiments (such as SAMBA, ARCANE-Eurofloat, ACCE), a new type of data is now available: positions of floats drifting at depth in the ocean. Unlike other data, mainly Eulerian, these ones are Lagrangian: the measuring instrument move in the flow. I will present methods and results about 4D-Var assimilation of Lagrangian data in the OPAVAR ocean model: implementation, sensitivity studies, assimilation of noisy observations, comparison with a classical method, complementarity with temperature data.

IC/MP102/015: Complexity of high-dimensional problems.

Organiser: Josef Dick (UNSW Asia, Singapore)
Co-organiser: Frances Kuo (University of New South Wales, Australia)

Tractability of high dimensional problems is an important criterion for deciding whether a problem can be solved within a reasonable time and effort. High dimensional problems occur often in applications and provide many challenging tasks even for nowadays computers. Hence the analysis of the inherent complexity of high dimensional problems becomes an interesting important topic.

Generalized tractability of multivariate problems. **Henryk Woźniakowski** (University of Warsaw, Poland) IC/MT1293/015

There is an increasing interest in solving multivariate problems of d variate functions with huge d. In this case, it is necessary to study how the errors of algorithms also depend on d. Polynomial tractability requires that the minimal error of algorithms using n function values or linear functionals depends at most polynomially on d and go to zero polynomially in n^{-1}. Generalized tractability may relax this requirement by admitting more than polynomial dependence which is, however, non-exponential.

We show for selected multivariate problems, such as integration and approximation, necessary and sufficient conditions for generalized tractability in terms of the properties of the underlying spaces defining the problem.

The worst-case error of (t,s)-sequences for integration in certain Hilbert spaces. **Peter Kritzer** (Universität Salzburg, Austria), Friedrich Pillichshammer (Universität Linz, Austria) IC/MT1165/015

We study the worst case error for quasi-Monte Carlo integration of functions from certain weighted Hilbert spaces which are based on Walsh functions. It has been shown recently that this worst case error is closely linked to a measure for the irregularity of distribution of a point set in the s-dimensional unit cube, namely the so-called dyadic diaphony as introduced by Hellekalek and Leeb in 1997. It is known that a sequence of points in $[0,1)^s$ is uniformly distributed modulo one if and only if the dyadic diaphony of the first N elements of the sequence converges to zero as N goes to infinity. A well-known example of such uniformly distributed sequences are (t,s)-sequences as introduced by Niederreiter in 1987.

We give an overview of recent results, and discuss bounds on the worst case error in the Walsh Hilbert spaces using digital (t,s)-sequences for quasi-Monte Carlo integration. Concerning the connection of the worst case integration error to the dyadic diaphony, we use our results to show that the dyadic diaphony of the first N elements of certain (t,s)-sequences in base 2 is of order $O(2^t(\log N)^{s/2}/N)$.

Lattice rules for integration over $\mathbb{R}^s$. **Stephen Joe** (University of Waikato, New Zealand) IC/MT4865/029

There has been much work done on lattice rules for the numerical approximation of integrals defined over the s-dimensional unit cube. If the integration region happens to be $\mathbb{R}^s$, it is quite common to apply some transformation to map $\mathbb{R}^s$ to the unit cube in order to make use of these lattice rules.
However, there do exist lattice rules for $\mathbb{R}^s$. For integrals over this unbounded region, the natural question that arises is whether such lattice rules have merit for the approximation of these integrals.

This talk is based on a joint work with Vasile Sinescu. We review some known results for these lattice rules and present some new preliminary theoretical results based on Fourier transforms and reproducing kernel Hilbert spaces.

QMC in multilevel Monte Carlo path simulation. **Michael Giles** (University of Oxford, UK) IC/MT5059/015

In this talk I will discuss the use of rank-1 lattice rules to further improve the computational complexity of multilevel Monte Carlo path simulation. Of particular interest is the fact that the QMC approach yields significant benefits on the coarsest (low-dimensional) levels, but very little benefit on the finest (high-dimensional) levels for which the multilevel technique has apparently already extracted most of the low-dimensional content.

IC/MP102/015: Complexity of high-dimensional problems. #2

Organiser: Josef Dick (UNSW Asia, Singapore)
Co-organiser: Frances Kuo (University of New South Wales, Australia)

(For abstract, see session #1 above.)

Randomized algorithms and complexity for elliptic PDE. **Stefan Heinrich** (TU Kaiserslautern, Germany) IC/MT1256/015

We study the randomized information complexity of elliptic partial differential equations with smooth coefficients in smooth domains D of R^d. The right hand side is supposed to belong to the Sobolev space $W_p^r(D)$, the solution is sought on a submanifold M of D, and the error is measured in the norm of $L_p(M)$, where $r \in N$ and $1 \le p < \infty$. We obtain matching up to logarithmic factors upper and lower bounds. The results extend previous investigations of the $p = \infty$ case.
We discuss algorithms for special cases that reach the optimal rates. They involve, in particular, multilevel Monte Carlo methods for approximating weakly singular operators and their use in connection with Green's functions.

A new quadrature using integration lattices. **Xiaoyan Zeng** (Illinios Institute of Technology, USA) IC/MT1345/015

We propose a new quadrature rule via approximating Fourier coefficients of variable transformed integrand with multidimensional integration lattice. The error analysis is derived for the proposed rule. A comparison is done between the new rule and the periodizing transformation methods. It shown that the new rule improves the periodizing transformation methods.

In the last part, we provide a semi-optimal quadrature for weighted integrals whose integrand is in Banach space.

This is joint work with Fred J. Hickernell and Rong-Xian Yue.

Efficient randomized algorithm for L_∞ approximation over reproducing-kernel Hilbert spaces. **Grzegorz Wasilkowski** (University of Kentucky, USA) IC/MT1070/015

In this talk we will present a randomized algorithm for approximating functions from reproducing kernel Hilbert spaces with the error measured in L_∞-norm. Although the algorithm uses only function values, it enjoys the same rate of convergence as the optimal algorithm that uses optimal linear functionals for L_∞-approximation in the deterministic worst case setting.

Algorithms for L_∞ approximation in the worst case setting. **Frances Kuo** (University of New South Wales, Australia) IC/MT940/021

This is a joint work with Grzegorz Wasilkowski and Henryk Woźniakowski. We consider the problem of function approximation, with the error measured in L_∞-norm and analyzed in the worst case setting. Our aim is to establish how powerful (in terms of the rate of convergence) an algorithm which uses only function values can be, compared to the optimal algorithm that uses arbitrary linear functionals.

In this talk I will present general multilevel algorithms that

are half as powerful as the optimal algorithm, under certain assumptions on the function space. In the special case of weighted Korobov spaces, I will show that lattice rule algorithms can be tailored to further reduce this gap in power.

IC/MP319/015: Current advances in domain decomposition methods and an outlook into the future.

Organiser: Martin Gander (Université de Genève, Switzerland)
Co-organiser: Victorita Dolean (Université de Nice Sophia Antipolis, France)

Classical domain decomposition methods like the overlapping Schwarz method or Schur complement methods have reached a great level of maturity toward the end of the 20th century. Research in Domain Decomposition methods has however not decreased over the last decade, on the contrary. New methods have been developed with significantly enhanced performance, and because of the current hardware development, parallel computing is of more importance than ever before. If you are interested in getting an overview on recent developments in domain decomposition methods, this minisymposium is for you. Speakers will present new domain decomposition methods for evolution problems, in space-time or purely in time, new coupling conditions between subdomains for better performance or for nonconforming meshes, new finite element tearing and interconnect (FETI) variants, and will give an outlook into the future on how domain decomposition methods can be used to achieve petascale performance.

Dynamic contact problems with different time and length scales. **Corinna Hager** (Universität Stuttgart, Germany), Barbara Wohlmuth (Universität Stuttgart, Germany) IC/MT4213/015

Nonlinear frictional contact problems are still a challenging task both from the mathematical and engineering point of view, for example in the simulation and design of car tires. In this case, the additional difficulty occurs that the fine structure of the tire profile needs to be resolved accurately enough to analyse the evolution of the contact stresses and the temperature during rolling contact. To get an accurate result without unnecessary computational effort, the actual contact zone is to be simulated with a finer time resolution than the rest of the tire.

In this report, we consider an efficient and stable numerical algorithm for dynamical contact problems with different length scales in the time and space domain. We employ nonconforming overlapping domain decomposition in space to resolve details of the domain boundary by a fine mesh; further we are able to choose the time scale on the subdomain independent of the one of the coarse domain. We analyse different ways of coupling between the coarse and the fine grid in order to separate the subproblems.

The resulting frictional contact problem is solved by a primal-dual active set strategy which can be modified to result in an energy-conserving robust algorithm with good results for the contact stresses. Numerical results containing Coulomb friction and non-linear material laws illustrate the behavior of the scheme.

This work was supported in part by Manufacture Française des Pneumatiques Michelin.

Optimized Schwarz methods. **Martin Gander** (Université de Genève, Switzerland) IC/MT4990/029

Optimized Schwarz methods have been developed over the last decade for three reasons: to obtain Schwarz methods which converge without overlap, to obtain convergent Schwarz methods for physical problems where the classical Schwarz method is not convergent, and to enhance the converge speed of Schwarz methods in general. All this is achieved in optimized Schwarz methods by replacing the Dirichlet transmission conditions from the classical Schwarz method by differential transmission conditions adapted to the physics of the underlying problem. I will give an introduction to this subject with examples of elliptic and time dependent problems, which illustrate the effectiveness of this new approach. I will conclude with two important open research problems in optimized Schwarz methods.

The relation between optimized Schwarz methods for scalar and systems of partial differential equations. **Victorita Dolean** (Université de Nice Sophia Antipolis, France), Martin Gander (Université de Genève, Switzerland) IC/MT3666/015

Schwarz algorithms experienced a second youth over the last decades, when distributed computers became more and more performant and available. Fundamental convergence results for the classical Schwarz methods were derived for many partial differential equations. Optimized Schwarz methods have been developed for scalar partial differential equations in order to achieve high performance by using transmission conditions between subdomains adapted to the physical problem solved, and are convergent even without overlap. More recently, Schwarz methods have also been extended to systems of equations, and it was found that even the classical Schwarz method converges without overlap in certain cases. Using Maxwell's equations and their equivalence to associated scalar partial differential equations, we show why the classical Schwarz method converges without overlap in this case, by proving that it is equivalent to a simple optimized Schwarz method for a scalar equation. Using this link, we develop transmission conditions with better performance than just exchanging information following the characteristics for systems of hyperbolic partial differential equations.

Parareal in-time algorithm for fast resolution of PDEs. **Yvon Maday** (Université Pierre et Marie Curie, France) IC/MT3009/015

The parareal in time algorithm allows to perform parallel computations over different processors by decomposing the time evolution interval into non overlapping slabs. The initial values at the beginning of each slab is upgraded through a kind of predictor corrector iterative method.

After presenting the basics of the method, we shall present different realizations where the algorithm is either performed alone or coupled with some other iterative approaches like domain decomposition or optimal control techniques.

An important aspect of the method is related to the choice of the predictor, this aspect will be discussed together with the definition of appropriate combination of the predictor and corrector as far as stability issues are involved.

IC/MP319/015: Current advances in domain decomposition methods and an outlook into the future. #2

Organiser: Martin Gander (Université de Genève, Switzerland)
Co-organiser: Victorita Dolean (Université de Nice Sophia Antipolis, France)

(For abstract, see session #1 above.)

Scalable solver software from the DOE SciDAC program. **David Keyes** (Columbia University, USA) IC/MT2800/015

Towards Optimal Petascale Simulations (TOPS) is a scalable solver software project based on domain decomposed parallelization and sponsored by the U.S. Department of Energy to research, implement, and support in collaborations with scientific users an open-source package for large-scale discretized PDE problems. Current applications include fusion reactor and accelerator modeling and design, flows in porous media, and quantum chromodynamics. Optimal complexity methods, such as multigrid/multilevel preconditioners, keep the time spent in dominant algebraic kernels close to linear in discrete problem size as the applications scale on massively parallel computers. Krylov accelerators and Jacobian-free variants of Newton's method, as appropriate, are wrapped around the multilevel methods to deliver robustness in multirate, multiscale coupled systems, which are solved either implicitly or in more traditional forms of operator splitting. The TOPS software framework is being extended beyond direct computational simulation to computational optimization, including design, control, and inverse problems. We outline the capabilities TOPS offers to high-end simulations generally, and illustrate on applications.

TOPS includes co-principal investigators at Argonne National Laboratory, Lawrence Berkeley National Laboratory, Lawrence Livermore National Laboratory, Sandia National Laboratories, Columbia University, the University of California at Berkeley and at San Diego, the University of Colorado at Boulder, and the University of Texas at Austin, and is led by the speaker.

Exact and inexact FETI-DP algorithms with applications to elasticity. **Axel Klawonn** (Universität Duisburg-Essen, Germany), Patrizio Neff (TU Darmstadt, Germany), Oliver Rheinbach (Universität Duisburg–Essen, Germany), Stefanie Vanis (Universität Duisburg–Essen, Germany) IC/MT3121/015

In this talk, first an introduction to exact dual-primal FETI methods willbe given together with a motivation for the need of inexact methods if tens of thousands of processors or even more are used. An algorithmic framework for inexact FETI-DP methods will be presented; theoretical and numerical results will be shown for standard linear elasticity problems. New results of our ongoing research on FETI-DP algorithms for a linear elasticity problem with non-constant coefficientswill be also presented. This problem is part of a non-linear, coupled, micromorphic model for the description of foam or bone substitution materials.

FETI-DP and BDDC preconditioners for spectral-element discretizations of elliptic problems in 2D. **Luca Pavarino** (Università degli Studi di Milano, Italy), Axel Klawonn (Universität Duisburg-Essen, Germany), Oliver Rheinbach (Universität Duisburg–Essen, Germany) IC/MT2860/015

Domain decomposition methods of the FETI-DP and BDDC families, recently developed for standard finite element discretizations, are here extended to tensorial spectral elements discretizations based on GLL quadrature. In spite of the more severely ill-conditioned discrete systems, the resulting preconditioners are parallel and scalable, since their convergence rate is independent of the number of subdomains and only logarithmically dependent on the polynomial degree and the number of elements per subdomain. The results of numerical tests on parallel machines confirm these conclusions for scalar and vector elliptic problems in the plane.

Primal- and dual-interface concentrated iterative substructuring methods. **Ulrich Langer** (Universität Linz, Austria), Sven Beuchler (Universität Linz, Austria), Tino Eibner (TU Chemnitz, Germany) IC/MT1696/015

This talk is devoted to the fast solution of interface-concentrated finite-element equations. The interface concentrated finite element schemes are constructed on the basis of a non-overlapping domain decomposition where a conforming boundary concentrated finite element approximation is used in every subdomain. Similar to the boundary element domain decomposition method the total number of unknowns per subdomain behaves like $O((H/h)^{(d-1)})$, where H, h, and d denote the usual scaling parameter of the subdomains, the average discretization parameter of the subdomain boundaries, and the spatial dimension, respectively. We propose and analyze primal and dual substructuring iterative methods which asymptotically exhibit the same or at least almost the same complexity as the number of unknowns. In particular, the so-called All-Floating Finite Element Tearing and Interconnecting solvers are highly parallel and very robust with respect to large coefficient jumps.

02: Numerical Analysis, Contributed Talks

IC/CTS4927/02: **Computation and designs.**

Organiser: Carlos deMoura (UERJ, Brazil)

New asymptotic estimates for spherical designs. **Andriy Bondarenko** (Kyiv University, Ukraine), Maryna Viazovska (TU Kaiserslautern, Germany) IC/CT1308/022

Let S^n be the unit sphere in $\mathbb{R}^{n+1}$. The set of vectors $\vec{x}_1, \dots, \vec{x}_N \in S^n$ is called a *spherical t-design* if

$$\frac{1}{mes\, S^n} \int_{S^n} p(\vec{x})\, \mathrm{d}\vec{x} = \frac{1}{N} \sum_{i=1}^{N} p(\vec{x}_i)$$

for all algebraic polynomials in $n+1$ variables and of degree at most t (see[1]). The low bound for cardinality $N = N(n,t)$ of spherical t-designs

$$\begin{cases} N(n,t) \geq \binom{n+k}{n} + \binom{n+k-1}{n} & \text{for } t = 2k, \\ N(n,t) \geq 2\binom{n+k}{n}, & \text{for } t = 2k+1, \end{cases}$$

is also proved in [1], that implies $N(n,t) \geq c(n)t^n$. It is also known [2] that $N(n,t) < +\infty$ for each n and t. For each fixed $n \in \mathbb{N}$ the upper bounds $N(n,t) \leq C(n)t^{\alpha_n}$, $t \to +\infty$, where $\alpha_n = O(n^4)$, $\alpha_n = O(n^3)$, $\alpha_n = (n^2+n)/2$ are proved in [3], [4] and [5] respectively. Our main result is as follows.

Theorem *Let a_n be the sequence defined by*

$$a_1 = 1, \quad a_{2n} = a_{2n-1} + 2n, \quad a_{2n-1} = 2a_{n-1} + n, \quad n \in \mathbb{N}.$$

Then, for all $n,t \in \mathbb{N}$ we have $N(n,t) \leq C(n)t^{a_n}$, where $C(n)$ is a constant depending only on n.

Corollary *For all $n,t \in \mathbb{N}$ with $n \neq 1$, we have $N(n,t) \leq C(n)t^{\frac{3}{2}n\log_2 n}$.*

[1] Delsarte, P., Goethals, J.M. and Seidel, J.J.; Spherical codes and designs, Geom. Dedicata 6 (1977), pp.363–388.
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[4] Bajnok, B.; Construction of spherical t-designs. Geom. Dedicata 43 (1992) pp.167–179.
[5] Korevaar, J. and Meyers, J.L.H.; Sherical Faraday cage for the case of equal point charges and Chebyshev-type quadrature on the sphere, Integral Transforms Spec. Funct. 1993, pp.105–117.

On Wachspress pentagonal patches. **Aparajita Ojha** (IIIT Jabalpur, India) IC/CT3445/015

Wachspress initiated the study of rational basis functions for finite element which have emerged as interesting tools for surface generation with desired smoothness over a region which accept partition in to polygonal or curved elements. He has mainly studied the constructional aspects of rational basis function for functional approximation. Later Gout and other mathematicians studied the interpolatory and convergence properties of lower degree rational finite element and their application in solving second order boundary value problems. These functions exhibit elegant mathematical properties. Due to their mathematical properties Dahmen, Dikshit and Ojha (Computer Aided Geometric Design, 17(2000), 879-890.) studied Wachspress quadrilateral patches from CAGD point of view. In (H.P. Dikshit and A. Ojha, Computer Aided Geometric Design, 19(2002), 207-224) conditions under which a composite quadrilateral patch will be C^1 continuous, has been studied. Further a simple subdivision formula has also been obtained in (H.P. Dikshit and A. Ojha, Computer Aided Geometric Design, 20(2003), 395-399)In this talk we shall present the construction of a pentagonal Wachspress type quadratic rational finite element patches. Among other things we shall present a nonnegative basis for the surface modeling over pentagonal partitions. Further, we shall discuss their interpolatory properties for construction of boundary elements interpolation. We shall conclude by giving the conditions under which a composite Wachspress patch will be C^1. A few example composite surfaces will be demonstrated fro possible applications in Computer Aided Geometric Design and Geometric Modelling applications.

Connectedness of number theoretic tilings. **Nertila Gjini** (University of New York, Tirana, Albania) IC/CT632/015

A non-empty set in $\mathbb{R}^n$ is called a *tile* if it coincides with the closure of its interior. If a finite set of tiles and their translations covers the space $\mathbb{R}^n$ without overlapping, then we say it forms a *tiling*. We study the connectedness of Pisot dual tilings which play an important role in the study of β-expansion, substitution and symbolic dynamical system. It is shown that each tile generated by a Pisot unit of degree 3 is arcwise connected. This is naturally expected since the digit set consists of consecutive integers. However surprisingly, we found families of disconnected Pisot dual tiles of degree 4. We proved that each tile of a tiling is connected or disconnected having infinitely many components. Also we give a simple necessary and sufficient condition for the connectedness of the Pisot dual tiles of degree 4. As a byproduct, a complete classification of the β-expansion of 1 for quartic Pisot units is given.

A strategy for parallel implementation of finite-difference schemes associated to evolution PDEs. **Carlos deMoura** (UERJ, Brazil), Maria Clícia Stelling deCastro (Universidade do Estado do Rio de Janeiro, Brazil), Vinícius Buçard deCastro (Universidade do Estado do Rio de Janeiro, Brazil) IC/CT2735/012

In the framework of parallel numerical treatment of PDEs, stationary (or time-frozen) equations have much more results available than the evolution (or time dependent) ones. This is justified as computer simulation of time flow, an intrinsically sequential phenomenum, leads naturally to a sequential algorithm, thus inhibiting any concurrency search. Among different approaches to circumvent this deadlock, the ones by Douglas *et al.* (frequency domain) and J.-L. Lions *et al.* (iterations), cf. [1,2], are worth mentioning.

The time-stepping strategy for PDEs is based on the fundamental semi-group property, sequentially read as:

$$u(t+\tau) = S(t)\big[S(\tau)\,u(0)\big]\,,$$

while its parallel view looks as

$$u(t+\tau) = \big[S(t)\,S(\tau)\big]\,u(0)\,,$$

which, for $t_n := n\Delta t$, gives

$$u(N\Delta t) = \big[S(t_{N-1})\,S(t_{N-2})\,\ldots\,S(t_0)\big]\,u(0)\,.$$

While looking at finite-difference schemes (FDS), replacement of the sequential view by the parallel one is equivalent to exchanging matrix–vector and matrix–matrix multiplications. But these latter can be carried out in parallel for linear problems. For any explicit FDS, this strategy, herein proposed and called *matrix-multiply method* (M^3), presents a speed-up of order $(2\ell\log_2 P)/P$ for P^2 active processors and ℓ the associated matrix half-band.

We emphasize:

- M^3 preserves all FDS stability and accuracy properties;
- all (space or time) mesh adaptive procedures may be kept along;
- speed-up estimate holds despite the filling caused by multiplications;
- Strassen-like product schemes lead to computer time improvement.

Experimental results are being conducted throughout different platforms. We should recall that part of this strategy was mentioned (for ODEs) almost 20 years ago by D.J. Evans, cf.[3].

[1] Douglas, J. (Jr.) *et al.*; Approximation of Scalar Waves in the Space–Frequency Domain. Math. Models Meth. Appl. Sci., 4, pp.509–531, 1994.
[2] Lions, J.-L. *et al.*; Résolution d'EDP par un schéma en temps "pararéel". C. Rendus Ac. Sc. Paris, 332(I), An. Numérique, pp.661–668, 2001.
[3] de Moura, C.A.; Parallel Algorithms for Differential Equations — a Survey. ch.10, pp.279–313. In *Models for Parallel and Distributed Computation: Theory, Algorithmic Techniques and Applications*, Appl. Opt. Series, V.67, R. Correa *et al.* (Eds.), Kluwer Ac. Publ., 2002.

Finite-element approximation to the equation of motion arising in Oldroyd model. **Amiya Pani** (IIT Bombay, India) IC/CT2907/025

Newton's model of incompressible viscous fluid is described by the wellknown Navier–Stokes equations. This has been a basic model for describing flow at moderate velocities of majority of viscous incompressible fluids encountered in practice. However, models of viscoelastic fluids have been proposed in the mid twentieth century which take into consideration the prehistory of the flow and are not subject to Newtonian flow. One such model was proposed by J.G. Oldroyd and hence, it is named after him. The equation of motion in this case gives rise to the following integro-differential equation

$$\frac{\partial u}{\partial t} + u\cdot\nabla u - \mu\Delta u - \int_0^t \beta(t-\tau)\Delta u(x,\tau)\mathrm{d}\tau + \nabla p = f(x,t)\,,\ x\in\Omega, t>0\,,$$

and incompressibility condition

$$\nabla \cdot u = 0\,,\ \ x \in \Omega, t > 0\,,$$

with initial condition

$$u(x,0) = u_0, u = 0,\ x \in \partial\Omega, t \geq 0\,.$$

Here, Ω is a bounded domain in $\mathbb{R}^d$ $(d = 2,3)$ with boundary $\partial\Omega$, $\mu > 0$ and the kernel $\beta(t) = \gamma exp(-\delta t)$, where both γ and δ are positive constants.

With a brief discussion on existential analysis, in this talk we concentrate on the finite element Galerkin method for the above system under realistically assumed regularity on the exact solutions. Since the problem is an integral perturbation of the Navier–Stokes equations, we would like to discuss *how far the results on finite element analysis for the Navier–Stokes equations can be carried over to the present case.*

Umbrella based triangulation of regular parametric surfaces. **Victoria Hernández Mederos** (ICIMAF, Havana, Cuba) IC/CT5068/020

IC/CTS4610/02: Factorizations and splittings.

Organiser: Martin Gutknecht (ETH Zürich, Switzerland)

Sparse direct factorizations based on unassembled hyper-matrices. **Paolo Bientinesi** (Duke University, USA), Victor Eijkhout (University of Texas at Austin, USA), Jason Kurtz (University of Texas at Austin, USA), Robert van de Geijn (University of Texas at Austin, USA) IC/CT252/020

This work is motivated by the observation that, for highly dynamic applications, traditional sparse direct solvers address the wrong problem. Such methods have focused on the efficient solution of an individual linear system, stored as a matrix in any traditional format, by manipulating the connectivity graph of the discretized domain and ordering degrees of freedom optimally.

In the setting of a FEM application with local mesh refinement and unrefinement, a factorization of a given linear system may already exist. It is the *updated* linear system of the (un)refined mesh for which a factorization must be computed in the least amount of time. That is, only parts of the matrix affected by refinement and/or unrefinement need to be updated. This observation holds the promise of a tremendous reduction in the cost of an individual refinement step.

We argue that traditional matrix storage schemes, whether dense or sparse, are a bottleneck, limiting the potential efficiency of the solvers. We propose a new data structure, the *Unassembled Hyper-Matrix* (UHM), which preserves useful information that can be provided by the application, and that can make the solver, as well as various other operations on the matrix, more efficient. In particular, this can be used to implement an efficient sparse direct solver for hp adaptive finite element problems.

On Hermitian and skew-Hermitian splitting iteration methods. **Zhong-Zhi Bai** (Chinese Academy of Sciences), Gene Golub (Stanford University, USA), Chi-Kwong Li (College of William and Mary, USA) IC/CT2784/020

The Hermitian and skew-Hermitian splitting (HSS) iteration scheme is an efficient and practical method for solving large sparse non-Hermitian system of linear equations. In this talk, after reviewing the HSS iteration method and its basic convergence theory for non-Hermitian positive definite matrices, we give a sufficient and necessary condition for guaranteeing its convergence for nonsingular and non-Hermitian positive semidefinite matrices. We then discuss the semi-convergence property of the HSS iteration method and derive a sufficient and necessary convergence condition for singular and non-Hermitian positive semidefinite matrices.

According to the optimal iteration parameter involved, we first compute it exactly for real two-by-two matrices, and then compute it exactly for special block two-by-two matrices. These formulas are used to give estimation for the optimal iteration parameter of HSS iteration method for general non-Hermitian matrices. Finally, some numerical results are used to examine the effectiveness of the HSS iteration method with the exact or the estimated optimal iteration parameter.

This talk includes works jointly finished with Prof. Gene H. Golub and Prof. Chi-Kwong Li.

Application of operator splitting in the solution of reaction–diffusion equations. **Tamas Ladics** (Budapest University of Technology and Economics, Hungary) IC/CT3117/015

Operator splitting is a widely used method in the numerical solution of partial differential equations (see: Marchuk, G.I., 1968: Some application of splitting-up methods to the solution of mathematical physics problems. *Applik. Mat.*, 13.). It has fruitful applications in for modeling of air pollution transport or in the solution of reaction-diffusion problems (see: Tamas Ladics, 2005: The analysis of the splitting error for advection-reaction problems in air pollution models. *Idojaras, Quarterly Journal of the Hungarian Meteorological Service*, Vol.109, No. 3, pp.173–188).

Operator splitting by its nature is convenient to implement on parallel computers. A comparison of the different splitting techniques in the solution of 1 and 2 dimensional reaction-diffusion equations is made. The process of the solution is a composition of certain splitting procedure and a given numerical method. We study the interaction between the different splitting procedures and different numerical schemes. The order of the convergence of this composed method is calculated. The error of the approximate solution is characterized as a function of the applied splitting and numerical scheme.

Pseudo-spectral finite-difference method for solving a 3D dual-phase-lagging heat-transport equation in a microscale thin film. **Sayed Hodjatollah Momeni-Masuleh** (Shahed University, Iran) IC/CT797/015

Non-Fourier microscale effects are significant during the rapid heating of metallic substrates. The heat transport equation is different from the traditional heat diffusion equation since a second-order derivative of temperature with respect to time and a third-order mixed derivative of temperature with respect to space and time are introduced. This study aims to develop a time dependent pseudospectral-finite difference scheme for solving a 3D dual-phase-lagging heat transport equation in a microscale thin film. The scheme uses periodic pseudospectral discretization in space and a fully second-order finite difference discretization in time. The scheme is illustrated by numerical examples. Comparisons are made with available literature.

Practical Newton-like acceleration algorithms for nonlinear system at singular roots. **Zorana Lužanin** (University of Novi Sad, Yugoslavia), Nataša Krejić (University of Novi Sad, Yugoslavia) IC/CT826/015

A new modification of Broyden, discrete Newton, column-updating and Thomas methods for solving singular system of nonlinear equations is introduced. Quasi-Newton methods are slower (linear or sublinear), if the Jacobian is singular at the solution. With the new modification convergence becomes linear or superlinear. The theory and method are illustrated by several examples.

IC/CTS4630/02: Numerical methods for differential equations.

Organiser: Jae-Hun Jung (Univ. Massachusetts at Dartmouth, USA)

Numerical consistency of high-order Galerkin-type polynomial methods for the reduction of round-off errors. **Jae-Hun Jung** (Univ. Massachusetts at Dartmouth, USA), Sigal Gottlieb (Univ. Massachusetts at Dartmouth, USA) IC/CT3060/025

Multi-domain penalty Galerkin polynomial spectral methods are well known to yield increasing order of accuracy for the smooth problems as the polynomial order is increased. Depending on the form of the penalty-type interface/boundary conditions there may exists a certain order of polynomial beyond which the spectral accuracy is no longer maintained but the round-off errors become dominant.

In this talk, we derive the general weak formulation using penalty-type interface/boundary conditions in multi-domain penalty Galerkin spectral method. We show that depending on the particular form of the penalty term, the derived multi-domain penalty Galerkin spectral method can be made equivalent to the discontinuoud Galerkin method. Our numerical results demonstrate that for some choices of penalty terms, an inconsistency in the techniques for evaluating the integrals may result in increased sensitivity to round-off errors, whereas consistent evaluations of the mass and the load vector produce more accurate results.

We also present a technique for reducing the sensitivity of round-off errors for high order polynomial Galerkin methods by exploiting their spectral convergence property. The expansion coefficients of the smooth solution obtained by the these methods decays exponentially. This decay rate deteriorates when the round-off errors become dominant. By truncating them properly, in a way which mimics spectral decay, we resolve the "exponential" error growth for high order polynomials. Some numerical experiments will be presented to show the high accuracy of the proposed method.

Miminal stabilization of discontinuous Galerkin finite-element methods for hyperbolic problems. **Benjamin Stamm** (École Polytechnique Fédérale de Lausanne, Switzerland), Erik Burman (École Polytechnique Fédérale de Lausanne, Switzerland) IC/CT1947/026

We consider a discontinuous Galerkin finite element method for the advection–reaction equation in two space–dimensions. For polynomial approximation spaces of degree greater than or equal to two on triangles we propose a method where stability is obtained by a penalization of only the upper portion of the polynomial spectrum of the jump of the solution over element edges. We prove stability in the standard h-weighted graph-norm and obtain optimal order error estimates with respect to mesh-size.

An application of some high-order operator-splitting methods to systems of stiff differential equations. **Francisco Sánchez-Bernabe** (Universidad Autonoma Metropolitana Iztapalapa, Mexico), Javier Salcedo-Ruiz (Instituto Politecnico Nacional, Mexico) IC/CT2589/025

In this work we compare operator splitting methods of high order that are applied to systems of stiff diffusion equations. In order to efficiently solve the resultant subproblems of these decomposition techniques is necessary to use implicit Runge-Kutta methods. Some operator splitting schemes were generated by applying Richardson extrapolation to lower order decomposition methods. It is known that, in this context, the accuracy of operator splitting schemes is reduced. However, we have observed that the order reduction is not very severe for high order operator splitting methods.

Numerical dissipativity of multistep methods for delay-differential equations. **Hongjiong Tian** (Shanghai Normal University, PR China) IC/CT1126/024

Dissipative differential equations have frequently appeared in the fields of physics, engineering, and biology. In this paper we investigate numerical dissipativity of linear multistep and one-leg methods applied to a class of dissipative delay differential equations. We show that for such class of dissipative systems these numerical methods are dissipative if and only if they are $A-$stable for ordinary differential equations. One numerical experiment is given to illustrate our result.

Long-memory Mori–Zwanzig models for the Euler equations. **Panagiotis Stinis** (Lawrence Berkeley National Laboratory, USA) IC/CT3020/025

A long memory model for dimensional reduction, known as the t-model, is derived through the Mori–Zwanzig formalism of irreversible statistical mechanics. The model is applied to the estimation of the rate of decay of solutions of the Burgers equation and of the Euler equations in two and three space dimensions. In the Burgers case, the model captures the rate of decay exactly. For the Euler equations in two space dimensions, the model preserves energy as it should. In three dimensions, we find a power-law decay in time and observe a temporal intermittency. The t-model is the first in a hierarchy of Mori–Zwanzig models.

This is joint work with A. Chorin, O. Hald and Y. Shvets.

Highly-efficient compact finite-difference methods for nonlinear partial differential equations. **Jichao Zhao** (INRIA, France) IC/CT2681/027

Multigrid method (MG) has been widely accepted as an efficient approach for solving linear elliptic partial differential equations. The multigrid method when combined with nested iteration, called Full Multigrid method (FMG), can solve linear matrix equations to the accuracy of the truncation error in a number of operations that is proportional to the number of unknowns. This powerful solver has a two-grid process, the fine-grid smooth and coarse-grid correction. To solve nonlinear partial differential equations, there are two basic approaches, Newton method and Full Approximation Scheme (FAS), to combine with the multigrid method, as demonstrated in Henson's overview (2000). Using higher order approximations in the fine-grid smooth or coarse-grid correction or both processes of the multigrid method provides a means of obtaining the same accuracy with much less computational time and amounts of storage compared with the common used second-order finite difference scheme. Schaffer (1985) and Burger and Fulton (1999) compared the three higher-order multigrid methods to solve linear elliptic partial differential equations: (i) smoothing with higher-order difference scheme via compact finite differ-

ence schemes (Mehrstellen Verfahren discretizations), (ii) iterated defect corrections with multigrid method used as an inner loop solver, and (iii) tau extrapolation, and they all concluded that the compact finite difference method is the most accurate and efficient one among these discretizations considered in their work.

In our work, we give the fourth-order compact finite difference scheme, combined with the FAS and Newton's method respectively, to solve nonlinear elliptic partial differential equations. We compare numerical results obtained by the compact finite difference method with the widely used second-order finite difference method, and the another higher-order method – iterated defect corrections, and draw the conclusion that the compact finite difference method combined with the multigrid method is a very efficient and accurate scheme for nonlinear elliptic partial differential equations. However, we must admit that it is quite complicated to generate compact finite difference schemes by hand, especially for general nonlinear partial differential equations or high dimensional problems, considering these higher-order schemes involve more grid points. To make life easier, we make a Maple package "CompactScheme" to generate these higher-order compact finite difference schemes for very general partial differential equations so that users can easily use them for their own purposes.

This is a join work with Dr. Jean-Antoine Désidéri and Alex Potapchik.

IC/CTS4603/02: Interpolation, quadrature, ODEs and integral equations.

Organiser: Leonid Knizhnerman (Central Geophysical Expedition, Russian Federation)
Co-organiser: Michael Minion (University of North Carolina, USA)

Choice of frequency interpolation nodes for solving a multi-frequency problem with a nonnegative definite operator. **Leonid Knizhnerman** (Central Geophysical Expedition, Russian Federation), Vladimir Druskin (Schlumberger Ltd., USA), Mikhail Zaslavsky (Schlumberger Ltd., USA) IC/CT2203/024

Let us have a family of equations:

$$(A + i\omega)u_\omega = \varphi, \qquad 0 < \omega_{\min} \le \omega \le \omega_{\max},$$

where A is a self-adjoint non-negative definite operator in a Hilbert space and φ is a nonzero vector. Given n, we wish to find basic frequencies ω_j, $1 \le j \le n$, such that u_ω can be well approximated by linear combinations of u_{ω_j}.

We have experimentally found out that good enough basic frequencies can be extracted from Zolotaryov's approximation to $\omega^{-1/2}$ on a bounded positive interval. The coefficients x_j of linear combinations can be obtained via solution of Galerkin type systems in the weighted spectral functional space:

$$(\lambda + i\omega)\sum_{j=1}^{n} x_j \frac{1}{\lambda + i\omega_j} - 1 \perp \frac{1}{\lambda + i\omega_k}, \qquad 1 \le k \le n.$$

Here $\lambda \ge 0$ represents the spectrum of A and the weight function is $\lambda^{-1/2}$.

The use of the real and imaginary parts of $\frac{1}{\lambda+i\omega_k}$ makes the convergence twice faster.

A hypothesis on the approximation error has been formulated. It is illustrated with the results of numerical experiments.

Accelerating the convergence of spectral deferred-correction methods for stiff ODEs and DAEs. **Michael Minion** (University of North Carolina, USA), Anita Layton (Duke University, USA), Jingfang Huang (University of North Carolina, USA), Jun Jia (University of North Carolina, USA) IC/CT4466/024

Spectral deferred correction methods (SDC) for ODEs have been shown to possess favorable accuracy and stability properties even for versions with very high order of accuracy. Unfortunately, for very stiff problems, SDC methods exhibit order reduction for a range of time-step values. I will show that for linear problems, the iterations in the SDC algorithm are equivalent to constructing a preconditioned Neumann series expansion for the solution of the standard collocation discretization of the ODE. I will explain the connection between order reduction and the convergence of this series. These observations motivate the use of Krylov subspace methods to accelerate the convergence of SDC for both ODEs and DAEs. The resulting methods possess increased stability and efficiency compared to the original SDC approach, and the acceleration effectively eliminates order reduction in the preliminary linear and nonlinear numerical experiments studied thus far.

Complexity of initial-value problems for ordinary differential equations of order-k. **Marek Szczęsny** (Akademia Górniczo-Hutnicza, Poland) IC/CT4083/015

We present results on the solution of initial-value problems for ordinary differential of order k. Our aim is to compute an ε-approximation to the solution. We study the dependence of the minimal error on the order k of the equation. We assume that the right-hand side function has r continuous bounded partial derivatives. We consider three models of computation: deterministic, randomized and quantum.

In the deterministic case we consider two types of information: standard information and linear one. For standard information, we show that the worst-case ε-complexity is $\Theta((1/\varepsilon)^{1/r})$, which is independent of k. Linear information is more powerful. We show that the ε-complexity in a class of equations is $\Theta((1/\varepsilon)^{1/(r+k)})$.

We also study possible advantages of randomized and quantum computing over deterministic computing. We show that a speed-up dependent on k is not possible in the randomized and quantum settings. We establish lower complexity bounds, showing that the randomized and quantum complexities are $\Theta((1/\varepsilon)^{1/(r+1/2)})$ in the randomized setting and $\Theta((1/\varepsilon)^{1/(r+1)})$ in the quantum setting. That is, they remain at the some level as for systems of the first order, no matter how large k is.

[1] Szczęsny M.; *Complexity of Initial-Value Problems for Ordinary Differential Equations of Order k*. Journal of Complexity, 22, **4** (2006), pp.514–532.
[2] Gońwin M., Szczęsny M.; *Randomized and Quantum Algorithms for Solving Initial-Value Problems of Ordinary Differential Equations of Order k*. In preparation.

Numerical methods for surface diffusion on elastically stressed solid surface. **Xiaofan Li** (Illinois Institute of Technology, USA) IC/CT4331/023

The surface diffusion of an axisymmetric solid, a whisker, subject to applied uniaxial stress, is studied numerically based on a new boundary integral formulation for periodic stress configurations. Efficient and accurate numerical methods for solving the boundary integral equation for elasticity and the severely stiff differential equations are presented. Numerical simulations of a fully nonlinear case are also presented, and evidences of singularity formation of the whisker are shown.

Numerical solution of integral equations using Legendre-wavelet functions. **Sohrab Rahbar** (Iran Research Organization of Science/Technology) IC/CT4974/023

Two methods for solving the linear and non-linear Fredholm integral equation of the second kind; i.e.,

$$f(x)-\lambda\int_a^b K(x,y)f(y)dy=g(x),\quad f(x)-\lambda\int_a^b K(x,y)F(f(y))dy=g(x),$$

are proposed. In order to solve the linear equation, the kernel $K(x,y)$ as well as the functions f and g are initially approximated through Legendre-wavelet functions. This leads to a system of linear equations whose solution provides a solution to the linear Fredholm integral equation.

In the second method for non-linear case, only the kernel $K(x,y)$ is approximated by Legendre-wavelet base functions. This leads to a separable kernel and makes it possible to employ a number of earlier methods in solving non-linear Fredholm integral equation with separable kernels. Another feature of the proposed method is that it finds the solution as a function instead of specific solution points, what is done by the majority of the existing methods.

A quadrature free convergent method for the numerical solution of linear Fredholm integral equations based on Hermit-spline interpolation. **Sedghat Shahmorad** (University of Tabriz, Iran) IC/CT603/023

In this paper we use the Hermite-spline interpolation in a special form for the numerical solution of linear Fredholm integral equations. We prove the convergence of this method as a main part of the paper and give an error bound for the error controlling of numerical results. Finally some numerical results are given to certify convergence and error bound of the method.

IC/CTS4926/02: Numerical linear algebra.

Organiser: Jan Mayer (Universität Karlsruhe, Germany)
Co-organiser: Martin Gutknecht (ETH Zürich, Switzerland)

ILU++: a new software package for solving sparse linear systems with iterative methods. **Jan Mayer** (Universität Karlsruhe, Germany) IC/CT1191/002

ILU++ is a new software package using a multilevel incomplete LU-factorization as a preconditioner. For better stability and sparsity, the factorization implements either pivoting by both rows and columns and/or sophisticated preordering and scaling techniques. Some of these techniques come from existing software packages (PARDISO, METIS), while others are new. ILU++ is written in C++ and fully templated, allowing for great flexibility. In particular, it can be easily integrated as a solver in other software.

A parallel Krylov–Schur implementation for large Hermitian and non-Hermitian eigenproblems. **Andrés Tomás** (Universidad Politecnica de Valencia, Spain), Vicente Hernández (Universidad Politecnica de Valencia, Spain), José Román (Universidad Politecnica de Valencia, Spain) IC/CT1524/012

Sorensen's implicitly restarted Arnoldi (IRA) algorithm is one of the most successful methods for finding a few eigenpairs of a large sparse matrix. The Krylov–Schur algorithm has been recently proposed by Stewart as an interesting alternative with two advantages over IRA. The first one is the ease of deflation of converged Ritz vectors, and the second one is the avoidance of the potential forward instability of the QR algorithm.

This work presents a new implementation of a Krylov–Schur eigensolver in SLEPc (Scalable Library for Eigenvalue Problem Computations), a software library for the solution of large, sparse eigenvalue problems on parallel computers. SLEPc can be used for the solution of problems formulated in either standard or generalized form, both Hermitian and non-Hermitian, with either real or complex arithmetic. It is built on top of PETSc (Portable, Extensible Toolkit for Scientific Computation) a parallel framework for the numerical solution of partial differential equations.

This Krylov–Schur implementation pursues numerical stability as well as parallel efficiency. The numerical stability of the implementation is assessed by an empirical test with a battery of about 200 public domain real-problem matrices.

The parallel performance analysis has been performed in a cluster platform with 55 nodes, computing a few extreme eigenpairs of large Hermitian and non-Hermitian problems. In particular, it has been compared with the IRA implementation from the ARPACK library and with the Arnoldi method with explicit restart from SLEPc. In addition, for Hermitian problems, it has been compared with several Lanczos variants with explicit restart from SLEPc.

Although the speed-up of this Krylov–Schur implementation is as good as the compared methods, the elapsed sequential time is lower, resulting in better overall performance.

Computing transfer function dominant poles of large-scale second-order dynamical systems. **Joost Rommes** (NXP Semiconductors, The Netherlands) IC/CT4569/020

A new algorithm for the computation of dominant poles of transfer functions of large-scale second-order dynamical systems is presented: Quadratic Dominant Pole Algorithm (QDPA). The algorithm works directly with the system matrices of the original system, so no linearization of the corresponding quadratic eigenvalue problem is needed. To improve global convergence, QDPA uses subspace acceleration, and deflation of found dominant poles is implemented in a very efficient way. The dominant poles and corresponding eigenvectors can be used to construct structure-preserving modal approximations, but also to improve reduced-order models computed by rational Krylov subspace methods, as is illustrated by numerical results. Generalizations to MIMO systems, higher-order systems and the computation of dominant zeros are also discussed.

Behaviour of the simple genetic algorithm. **Stefan Kotowski** (Polish Academy of Sciences, Poland) IC/CT4789/012

There will be presented the possibility of generating the limit distribiution of the simple genetic algorithms in optimal way, (possibly in one step). The formal construction of the best genetic algorithm as the idea for construction real genetic algorithm as the approximation the possibly best genetic algorithm will be presented.

A comparison between different bases in image reconstruction from non-uniform samples. **Reginaldo Santos** (Universidade Federal de Minas Gerais, Brazil) IC/CT2248/021

We present two methods based on the application of Conjugate Gradient method that use wavelets and shift invariant spaces bases. We give an efficient way of computing the products Ax and A^*y for each basis. We compare, experimentally, our approach for image reconstruction from nonuniform samples when using Fourier, D6 wavelets and uniform cubic splines bases.

Finite volume-element method for miscible displacement problem in porous media. **Sarvesh Kumar** (IIT Bombay, India) IC/CT2884/025

We present the finite volume element methods (FVEM) for incompressible miscible displacement problems in porous media. The miscible displacement in porous media is modeled by a nonlinear system of two partial differential equations, one is pressure equation and other is called concentration equation. For the approximation of pressure equation we use mixed FVEM and for approximating the concentration equation we apply the standard FVEM. Optimal error estimates are derived for velocity as well as concentration. Numerical results confirm the theoretical order of convergence.

IC/CTS4637/02: Numerical methods for elliptic pde's.

Organiser: Raffaello Seri (Università degli Studi dell'Insubria Varese, Italy)
Co-organiser: Zhongqing Wang (Shanghai Normal University, PR China)

Diaphonies on Sobolev classes of functions. **Raffaello Seri** (Università degli Studi dell'Insubria Varese, Italy) IC/CT4362/002

The aim of this paper is to provide a general way to build Koksma–Hlawka inequalities for integration of Sobolev functions through a sample of monte Carlo and quasi-Monte Carlo points. The technique is very general and can be applied, as an example, to the hypercube, the hypersphere and the disc. The bound in the inequality is given by the product of a term depending only on the function to be integrated (and on a pseudodifferential operator) and a term depending on the sample of points and given by a diaphony in the sense of Amstler and Zinterhof. It is also possible to give a general interpretation of these diaphonies as worst-case integration errors of quadrature rules. A consequence is that Giné Sobolev tests used in Statistics coincide with diaphonies appearing in Koksma-Hlawka inequalities based on pseudodifferential operators in the spirit of Cui and Freeden for the integration of Sobolev functions defined on compact Riemannian manifolds.

Work done in collaboration with Christine Choirat.

Weighted moving finite elements applied to reacting and non-reacting flow problems, including applications with remeshing and refining. **Abigail Wacher** (Finavera Renewables Ltd., Canada), Dan Givoli (Technion-Israel Institute of Technology) IC/CT932/002

Solving problems containing complex structures or moving shocks using standard methods can be computationally expensive, and using an adaptive mesh to *track* moving fronts and boundaries has been shown to provide cheaper and more accurate computations, making them a good candidate for solving large-scale problems in several areas in the Engineering Sciences.

Recently my work has focused on the development and implementation of a moving mesh technique called *String Gradient Weighted Moving Finite Elements* (suggested by K. Miller in 1997). I will introduce the method and present results to several systems of nonlinear partial differential equations, including a two dimensional model of a chemical reaction, the porous medium equation, and solutions to the dispersive and non-dispersive nonlinear shallow water equations.

Two deficiencies of the original SGWMFE method are (1) possible tangling of the mesh which causes the method's failure, and (2) no mechanism for global refinement when necessary due to the constant number of degrees of freedom. Recently the method has been extended in order to continue computing solutions when the meshes become too distorted, which happens quickly when the flow is rotationally dominant. Optimal rates of convergence are obtained when remeshing is applied. The method is also extended to include refinement to enable handling of new physical phenomena of a smaller scale which may appear during the solution process. It is shown that the errors in time are kept under control when refinement is necessary. Results of the extended method for some example problems of water hump release are presented.

Numerical solution of the dynamic problem of the elasticity theory in arbitrary shaped plane domain. **Galina Ribacova** (Moldova State University) IC/CT942/027

The large number of problems connected with numerical modeling of different physical processes leads to necessity of creation of effective methods of discretization of the computational fields with complicated shape. In order to solve this problem there are often used the methods based on application of the elliptical type partial differential equations for description of the interconnection between the computational (ξ, η) and physical (x, y) regions [1]. In present article the method of creating the regular two dimensional curvilinear grids based on the solution of the problem of longitudinal elastic plate deformation is presented. Mathematically the problem represents the system of partial differential equations of elliptic type – Lame's equations [2]. To formulate the problem let us consider the rectangular elastic plate. Let the rectangular uniform grid with the grid points $\left(x_i, y_j\right), x_i = ih_x, y_j = jh_y, i = \overline{0,n}, j = \overline{0,m}$, ($h_x = l_1/n, h_y = l_2/m$ – the steps of the grid on corresponding variable, l_1 and l_2 – the dimensions of rectangular plate) is marked on this plate. If now the plate is exposed to longitudinal deformation so as its boundaries take some given form (the form of boundaries of the region where the grid must be constructed), then the grid, which was marked on plate, will be deformed too. As a result of such deformation we obtain the unknown grid. The problem is solved numerically by means of finite difference method with second order accuracy on the rectangular grid that has been introduced above [3]. The developed algorithm was applied for discretization of the regions with complicated geometrical structures.

The finite-element method for a class of degenerate elliptic equations. **Hengguang Li** (Department of Mathematics, the Pennsylvania State, USA) IC/CT736/026

Consider the degenerate elliptic operator $\mathcal{L}_\delta := -\partial_x^2 - \frac{\delta^2}{x^2}\partial_y^2$ on $\Omega := (0,1) \times (0,l)$, for $\delta > 0, l > 0$. We prove well-posedness and regularity results for the degenerate elliptic equation $\mathcal{L}_\delta u = f$ in Ω, $u|_{\partial\Omega} = 0$ using weighted Sobolev spaces K_a^m. In particular, by a proper choice of the parameters in the weighted Sobolev spaces K_a^m, we establish the existence and uniqueness of the solution. In addition, we show that there is no loss of K_a^m-regularity for the solution of the equation. We then provide an explicit construction of a sequence of finite dimensional subspaces V_n for the finite element method, such that the optimal convergence rate is attained for $u_n \in V_n$, i.e., $||u - u_n||_{H^1(\Omega)} \leq C\dim(V_n)^{-\frac{m}{2}}||f||_{H^{m-1}(\Omega)}$ with C independent of f and n. Numerical results will be shown.

Mixed spectral method for 3D exterior problems using spherical-harmonic and generalized-Laguerre functions. **Zhongqing Wang** (Shanghai Normal University, PR China) IC/CT1528/014

In this talk, we develop the mixed spectral method for three-dimensional exterior problems, using spherical harmonic and generalized Laguerre functions. Some basic approximation results are established. The mixed spectral schemes are proposed for two model problems. Their convergences are proved. Numerical results demonstrate the efficiency of this new approach.

IC/CTS4925/02: Numerical methods for advanced applications.

Organiser: Manfred Trummer (Simon Fraser University, Canada)
Co-organiser: Vianey Villamizar (Brigham Young University, USA)

Optimized Schwarz methods for the spherical Laplacian with corners. **Sébastien Loisel** (Temple University, USA) IC/CT4513/027

Numerically solving the Laplace problem on the sphere is important in several fields, including meteorology. When the number of grid points is large, one possibility to solve the linear problem $Lu = f$ is to use an iterative method. One such method is the Schwarz iteration. Several difficulties are particular to the sphere. First, the spherical Laplacian is singular, so the Schwarz iteration does not converge in the traditional sense. Second, Optimized Schwarz Methods (OSM) (which replace the Dirichlet problem by a Robin or higher order problem) have difficulties dealing with corners and multiple intersections of subdomains. Third, coarse grid corrections are not well understood for OSM. Fourth, convergence results for OSM are not generally known for optimized parameter values. In this talk, we will address all of these issues.

Adaptive finite-element meshing scheme for the steady Navier–Stokes equations. **Hyung-Chun Lee** (Ajou University, Republic of Korea), Lili Ju (University of South Carolina, USA) IC/CT1886/027

A triangle mesh adaptivity algorithm for Navier–Stokes equations that combines *a posteriori* error estimate with centroidal Vorioni/Delaunay tessellations of domains in two demensions is proposed and tested. With *a posteriori* error estimate, mesh adaptativity algorithm has several desirable features. Errors are very well equidistibuted over the triangles. The achieved convergence rates are the best obtainable using Taylor-Hood finite elements.

Comparison of different methods applied to the solution of problems with non local boundary conditions. **Abdelaziz Chetouani** (Université Mohammed 1er Oujda, Morocco), Zakaria El Allali (Université Mohammed Premier Oujda, Morocco) IC/CT620/028

Non-linear equations with non-local boundary conditions are used to model several physical phenomena. An exhaustive description of the accuracy of such equations is given by Fairweather and Saylor. In this paper we give different methods for the numerical solutions of such equations. First, a family of numerical methods is developed for the numerical solution of a linear parabolic problem with boundary conditions containing integrals over the interior of the interval. The methods are seen to evolve from first- and second-order rational approximants to an exponential function in a recurrence relation. Global extrapolation procedures in space only and in both space and time are discussed. In the second part of this paper, we analyze a θ-method for the numerical solution of a semi linear parabolic problem with boundary conditions containing integrals over the interior of the interval, existence and convergence are proved for $\theta \leq \frac{1}{2}$; numerical application is given. in the last part of this paper a numerical comparison of the different methods is presented.

On the relation of topology and analysis in discrete mechanics. **Sigrid Leyendecker** (California Institute of Technology, USA), Michael Ortiz (California Institute of Technology, USA), Jerrold Marsden (California Institute of Technology, USA) IC/CT2076/028

Discrete mechanics can be understood as a discrete theory for the deformation of solids based on a discrete differential complex, thus the underlying (space-time)-domain is discrete *ab initio*. In contrast to the finite element approach, the emanating discretisation techniques are not based on the interpolation of nodal values where the appearing differential operators are applied to the interpolating shape functions, but the differential operators are discretised themselves and the corresponding discrete operators are applied directly to the nodal values. The resulting discrete problem is expressed in a manner formally identical to its continuous counterpart, exhibiting discrete analogues of whose properties.

Concepts of discrete calculus have been investigated in the context of vector field theories (see e.g. [1], [2]). However its extension to tensor field problems such as discrete elasticity is not straightforward. In particular for constrained problems, the design of stable approximation schemes with good convergence properties requires certain topological properties of the discrete domain as well as an analysis of the involved interpolation spaces, see [3]. The aim of the talk is to draw connections between the discrete topology and analysis in the regime of finite deformation of solids.

[1] A. Bossavit. "Discretization of Electromagnetic Problems". available via http://www.icm.edu.pl/edukacja/mat/DEP.php, 2001.
[2] M. Desbrun, A. Hirani, M. Loek, and J.E. Mardsen. "Discrete Exterior Calculus". *arXiv:math.DG/0508341*, August 2005.
[3] P. Hauret, E. Kuhl, and M. Ortiz. "Diamond elements: A finite-element/discrete mechanics approximation scheme with guaranteed optimal convergence in incompressible elasticity". *Int. J. Numer. Meth. Engng.*, accepted for publication, 2006.

Regularization in dynamic SPECT. **Manfred Trummer** (Simon Fraser University, Canada) IC/CT4804/015

Single photon emission computed tomography (SPECT) is a widely used technique in diagnostic nuclear medicine. In the static setting, a constant image is assumed during the data acquisition process. In many applications, for example in the study of Teboroxime cardiac images, the activity varies with time. Reconstructing this time-dependent activity is the goal of dynamic SPECT. The problem is highly underdetermined, and thus ill-posed. A-priori information and regularization techniques must be used in the solution. We will present an algorithm for this problem based on Kalman filtering.

Acoustic scattering from multiple complexly-shaped obstacles. **Vianey Villamizar** (Brigham Young University, USA), Sebastian Acosta (Brigham Young University, USA) IC/CT4443/025

In this work, we develop an explicit finite-difference time-dependent method, based on boundary conforming coordinates including grid line control, to numerically solve two-dimensional scattering problems in the presence of multiple obstacles exhibiting boundary singularities. It constitutes an extension of previous work for single scatterers. The development of these methods requires appropriate definitions of radiation conditions at artificial infinite boundaries, the generation of curvilinear coordinates with efficient grid line control on multiply connected regions with several holes, and the reformulation of the boundary value problem (BVP) in terms of the new curvilinear coordinates. The scatterers are arbitrarily located inside the physical domain. The grid generation algorithm is capable of increasing the distance between grid lines in certain regions, where the Courant-Friedrichs-Lewy (CFL) stability condition may be violated. Hence, there is no need to further reduce the time step to reach stability as long as the size of each cell is maintained above the limits of stability. The computational advantage of the novel numerical method is revealed by applying it to various multiple scatterer configurations.

IC/CTS4607/02: Numerical linear algebra.

Organiser: Winfried Grassmann (University of Saskatchewan, Canada)

Spectral analysis of the discrete Helmholtz operator preconditioned with a shifted Laplacian. **Martin van Gijzen** (TU Delft, The Netherlands) IC/CT3501/020

Shifted Laplace preconditioners have attracted considerable attention as a technique to speed up convergence of iterative solution methods for the Helmholtz equation. We present a comprehensive spectral analysis of the Helmholtz operator preconditioned with a shifted Laplacian. Our analysis is valid under general conditions. The propagating medium can be heterogeneous, and the analysis also holds for different types of damping, including a radiation condition for the boundary of the computational domain. By combining the results of the spectral analysis of the preconditioned Helmholtz operator with an upper bound on the GMRES-residual norm we are able to provide an optimal value for the shift, and to explain the mesh-depency of the convergence of GMRES preconditioned with a shifted Laplacian. We will illustrate our results with a seismic test problem.

Comparison of algorithms for large scale nonlinear eigenvalue problems. **Yusaku Yamamoto** (Nagoya University, Japan) IC/CT2855/020

Given an $n \times n$ matrix $A(\lambda)$ whose elements depend on a scalar parameter λ, we consider a problem of finding the values of λ such that the linear equation $A(\lambda)\mathbf{x} = \mathbf{0}$ has a nonzero solution $\mathbf{x}$. We compare three algorithms. The first one is to apply Newton's method to nonlinear simultaneous equations consisting of $A(\lambda)\mathbf{x} = \mathbf{0}$ and some normalization constraint on $\mathbf{x}$. In the second approach, we view $A(\lambda)$ as a constant matrix and compute the eigenvalue of this matrix with the smallest modulus, which we denote by $e(\lambda)$. Then the value of λ that satisfies $e(\lambda) = 0$ is the solution of the original nonlinear eigenvalue problem. The third approach is similar to the second one, except that the smallest singular value of $A(\lambda)$ is used instead of the eigenvalue. Once the nonlinear eigenvalue λ is found, the eigenvector $\mathbf{x}$ can be computed from the null space of $A(\lambda)$.

We applied these methods to a nonlinear eigenvalue problem arising from theoretical fluid dynamics. In this problem, $A(\lambda)$ is a nonsymmetric matrix of order 35,000 to 100,000 and the smallest positive eigenvalue is sought. Numerical experiments show that it is difficult to obtain the desired eigenvalue with Newton's method unless a good approximation to the corresponding eigenvector $\mathbf{x}$ is available. In contrast, with the second and third approach we were able to compute the desired eigenvalue successfully. The third approach was more efficient since for a nonsymmetric matrix, the singular values can be computed more cheaply than the eigenvalues.

We also propose a method that can compute the nonlinear eigenvalues in a specified region of the complex plane using techniques from complex analysis.

A parallel eigenvalue-problem solver for computational nano-electronics. **Maxim Naumov** (Purdue University, USA), Ahmed Sameh (Purdue University, USA) IC/CT4100/020

Computational nanoelectronics gives rise to many large sparse eigenvalue problems. The energy levels of a nanodevice constitute important parameters that are needed to describe electronic transport. The energy levels can be found by solving a Hermitian eigenvalue problem, in which the eigenvalues of interest lie in an interior interval in the spectrum around 0.

In this talk we will present an approach that consists of using diferent mappings in combination with the Trace Minimization algorithm to obtain the desired eigenpairs. We will comment on its advantages compared to standard eigenvalue solvers/packages such as Lanczos and PARPACK. Finally, numerical experiments will also be presented.

Multi-level iterative solvers for the edge finite-element solution of the 3D Maxwell equation. **Mike Botchev** (Universiteit Twente, The Netherlands), Oleg Nechaev (Novosibirsk State Technical University, Russian Federation), Ella Shurina (Novosibirsk State Technical University, Russian Federation) IC/CT3115/002

In the edge vector finite element solution of the frequency-domain Maxwell equations, the presence of a large kernel of the discrete rotor operator is known to ruin convergence of standard iterative solvers. We extend the approach of [1] and, using domain decomposition ideas, construct a multilevel iterative solver where the projection with respect to the kernel is combined with the use of a hierarchical representation of the vector finite elements.

The new iterative scheme appears to be an efficient solver for the edge finite element solution of the frequency domain Maxwell equations. The solver can be seen as a variable preconditioner and, thus, accelerated by Krylov subspace techniques (e.g. GCR or FGMRES). We demonstrate the efficiency of our approach on a test problem with strong jumps in the conductivity.

[1] R. Hiptmair. Multigrid method for Maxwell's equations. *SIAM J. Numer. Anal.*, 36(1):204–225, 1999.

An efficient numerical simulation method for railway vehicle-track dynamic interaction. **Akiyoshi Yoshimura** (Tokyo University of Technology, Japan) IC/CT2065/020

An efficient numerical simulation method for the railway vehicle-track dynamic interactions is described. Applying the finite element method for the rail modelled as an Euler beam, the following equations of motion are obtained.

$$M\ddot{\boldsymbol{u}} + C\dot{\boldsymbol{u}} + (K + K_t)\boldsymbol{u} = \boldsymbol{g}(t)$$

where $\boldsymbol{g}(t)$ contains the contact force between the wheel and the rail.

In the equation, the stiffness matrix can be expressed separately to the time-invariant term K and the time-dependent one K_t. Moreover, by investigating the linear algebraic structure of the model the time-dependent matrix K_t can be simply expressed as $K_t = \boldsymbol{a}_t\boldsymbol{a}_t^T$. The specially defined vector $\boldsymbol{a}_t$ has only a few nonzero elements. Applying the Newmark-β direct integration method for the numerical simulation, a linear system $A_t\boldsymbol{x}_t = \boldsymbol{b}_t$ is obtained. The A_t is a time-dependent, sparse symmetric positive definite matrix. The linear system has to be solved iteratively for each time step. Here A_t can be expressed as $A_t = A + \boldsymbol{a}_t\boldsymbol{a}_t^T$ and its time-dependent term $\boldsymbol{a}_t\boldsymbol{a}_t^T$ makes only a small change in the sparse matrix A_t. So the Sherman-Morrison formula can be used in the computation of the inverse A_t^{-1}, which enables a very efficient numerical simulation.

Spectra for infinite tridiagonal pseudo-Toeplitz matrices. **Winfried Grassmann** (University of Saskatchewan, Canada) IC/CT477/020

This talk deals with the eigenvalues and eigenvectors of a tridiagonal matrix A where the diagonally centred rows repeat after the first c rows. Let N be the dimension of A. It is shown that as $N \to \infty$, the set of eigenvalues becomes dense, except for up to a maximum of c isolated eigenvalues. We also show that the functions of A, such as e^A, can be expressed as the sum of an integral and terms deriving from the isolated eigenvalues. Numerical results for the case where all off-diagonal elements are positive are given, and they are encouraging. However, the number of points used to find the integral increases with the row number.

IC/CTS4609/02: Numerical linear algebra.

Organiser: Lev Krukier (Southern Federal University, Russian Federation)

Application of a new generalized conjugate-direction method to the linear complementarity problem. **Edouard Boudinov** (Fortis Bank, Brussels, Belgium), Arkadiy Manevich (Dnipropetrovs'k National University, Ukraine) IC/CT3452/020

In our presentation on GAMM–SIAM Conference on Applied Linear Algebra (Dusseldorf, 2006) a new generalized conjugate direction method for large non-symmetrical linear systems of equations has been proposed. The method unifies advantages of such powerful algorithms as the GMRES and CG methods. Similarly to GMRES and some other Krylov subspace methods for non-symmetrical matrices, the proposed algorithm uses an entire sequence of orthogonal basis vectors, obtained in the Arnoldi process. The Arnoldi process is also used for computing residuals with high accuracy. Unlike GMRES, the method employs explicitly computed conjugate (in a generalized sense) directions to determine iterates. Due to long recurrence and replacement of usual updating residuals with the Arnoldi orthogonalization, the algorithm is found to be very stable and efficient in solving large scale and/or ill-conditioned linear problems.

In this work the extension of the proposed algorithm to solving the linear complementarity problem (LCP) is presented. The problem consists in finding vector x that satisfies the following conditions :

$$\mathbf{A}x \geq \mathbf{b}, \quad x \geq \mathbf{c}, \quad (x - \mathbf{c}) \cdot (\mathbf{A}x - \mathbf{b}) = 0,$$

for a given matrix $\mathbf{A}$ and vectors $\mathbf{b}$ and $\mathbf{c}$.

To examine the efficiency of the proposed method we have applied it to a LCP of financial industry. The partial differential complementarity formulation of the financial option pricing problem leads to a sequence of LCPs. Since both the sequence and dimension of linear systems can be very large and the matrix may be ill-conditioned, the performance of the solver is of great importance. The efficiency of the method is compared with that of the most popular algorithm for solution of the LCP in option pricing – the projected successive overrelaxation method (PSOR).

Krylov-subspace methods for solving complex symmetric shifted linear systems. **Tomohiro Sogabe** (Nagoya University, Japan), Takeo Hoshi (Tottori University, Japan), Shao-Liang Zhang (Nagoya University, Japan), Takeo Fujiwara (University of Tokyo, Japan) IC/CT2614/020

We consider the solution of complex symmetric shifted linear systems of the form $(A + \sigma_k I)\mathbf{x}^{(k)} = \mathbf{b}$, for $k = 1, 2, \ldots, m$, where $A + \sigma_k I$ is a nonsingular N by N complex symmetric matrix with a scalar shift $\sigma_k \in \mathbb{C}$, and $\mathbf{x}^{(k)}, \mathbf{b}$ are complex vectors of length N. Such systems arise in large-scale electronic structure calculations (e.g., [3]), and there is a strong need for the fast solutions of the systems. In this talk, we present the recent development of Krylov subspace methods for solving this class of linear systems. The main talk will concern the shifted COCG method [3], the seed switching technique [2], and the shifted QMR_SYM method that is a variant of the QMR method for complex symmetric linear systems [1].

[1] R. W. Freund; Conjugate gradient-type methods for linear systems with complex symmetric coefficient matrices, SIAM J. Sci. Stat. Comput., 13(1992), pp.425–448.

[2] T. Sogabe, T. Hoshi, S.-L. Zhang, and T. Fujiwara; A numerical method for calculating the Green's function arising from electronic structure theory, to appear in Proc. of FCS2005, Springer-Verlag.

[3] R. Takayama, T. Hoshi, T. Sogabe, S.-L. Zhang, T. Fujiwara; Linear algebraic calculation of Green's function for large-scale electronic structure theory, Phys. Rev. B 73, 165108(2006), pp.1–9.

Preconditioned Krylov-subspace methods for the solution of least-squares problems. **Jun-Feng Yin** (National Institute of Informatics, Japan), Zhong-Zhi Bai (Chinese Academy of Sciences), Ken Hayami (National Institute of Informatics, Japan) IC/CT2396/020

We consider preconditioned Krylov subspace iteration methods, e.g., CG, LSQR and GMRES, for the solution of large sparse least-squares problems $\min \|Ax - b\|_2$, with $A \in \mathbf{R}^{m\times n}$, based on the Krylov subspaces $\mathcal{K}_k(BA, Br)$ and $\mathcal{K}_k(AB, r)$, respectively, where $B \in \mathbf{R}^{n\times m}$ is the preconditioning matrix. More concretely, we propose and implement a class of incomplete QR factorization preconditioners based on Givens rotations and analyze in detail the efficiency and robustness of the correspondingly preconditioned Krylov subspace iteration methods. A number of numerical experiments are used to further examine their numerical behaviour. It is shown that for both overdetermined and underdetermined least-squares problems, the preconditioned GMRES methods are the best for large, sparse and ill-conditioned matrices in terms of both CPU time and iteration step. Also, comparisons with the diagonal scaling and the RIF preconditioners are given to show the superiority of the newly-proposed GMRES-type methods.

[1] Z.-Z. Bai, I. S. Duff, and A. J. Wathen; A class of incomplete orthogonal factorization methods. I: methods and theo-

ries. BIT 41 (2001), pp. 53–70.
[2] Å. Björck; *Numerical Methods for Least Squares Problems*. SIAM, Philadelphia, 1996.
[3] K. Hayami and T. Ito; The solution of least squares problems using GMRES methods. Proc. of the Institute of Statistical Mathematics, 53 (2005), pp. 331-348, (in Japanese).

Computation of matrix functions in electromagnetic scattering using preconditioned rational Krylov subspaces. **Mikhail Zaslavsky** (Schlumberger Ltd., USA), Leonid Knizhnerman (Central Geophysical Expedition, Russian Federation), Vladimir Druskin (Schlumberger Ltd., USA) IC/CT3091/002

Preconditioning of Krylov subspaces for computing $f(A)b$ is a notoriously difficult problem except when $f(A) = A^{-1}$. We consider electromagnetic scattering problems where A is obtained from the FD discretization of Maxwell's system and we want to approximate $(A + \lambda I)^{-1}b$ for multiple values of the spectral parameter λ using a single rational Krylov subspace. We consider problems with $A = A_0 + A_1$, where A_0 is a "background" operator with easily computable resolvent and A_1 is an "anomaly" operator with local support. The main idea of our approach is the reduction of the subspace approximation from the entire computational domain to the support of A_1. Numerical examples for the 3D low frequency scattering problem show significant acceleration compared to the unpreconditioned subspace.

Skew-symmetric preconditioners for GMRES and BiCG. **Lev Krukier** (Southern Federal University, Russian Federation) IC/CT1928/020

The splitting of the initial matrix in its symmetric and skew-symmetric parts is applied. Then the upper and lower triangular parts of the skew-symmetric matrix are used as the basis for constructing special preconditioners for the solution of strongly nonsymmetric linear systems of equations.

Several theoretical results have been proved. Numerical experiments include the solutions of the strongly nonsymmetric linear equation systems arising from a central finite-difference approximation of the steady convection–diffusion equation with the Peclet numbers $Pe = 10^3$, 10^4 and 10^5. The relative performance of the methods with and without preconditioners for the popular GMRES(10) and BiCG methods have been tested and compared.

IC/CTS4615/02: Numerical linear algebra.

Organiser: Steven Leon (Univ. of Massachusetts at Dartmouth, USA)

Gram–Schmidt orthogonalization: 100 years and more. **Steven Leon** (Univ. of Massachusetts at Dartmouth, USA), Walter Gander (ETH Zürich, Switzerland) IC/CT2697/020

In 1907 Erhard Schmidt published a paper where he introduced an orthogonalization algorithm that has since become known as the classical Gram-Schmidt process (CGS). Schmidt claimed that his procedure was essentially the same as an earlier one published by J. P. Gram in 1883. The Schmidt version was the first to become popular and widely used. The two algorithms produce the same results when carried out in exact arithmetic, however, the Gram version, now known as the modified Gram-Schmidt process (MGS), produces superior results when carried out in finite precision arithmetic. In actuality, Gram rediscovered a method that first appears in an 1816 paper by P. S. Laplace. While the MGS algorithm has been around for almost 200 years, it is the Schmidt paper that led to the popularization of orthonormalization techniques. In celebration of the 100th anniversary of that paper, we present a comprehensive survey of the research on Gram-Schmidt orthogonalization and its related QR factorization.

Structured backward errors and pseudospectra of structured matrix pencils. **Rafikul Alam** (IIT Guwahati, India) IC/CT471/020

Structured pencils occur in many practical applications. Most often, the eigenvalues of structured pencils have certain spectral symmetries and it is very important to preserve these spectral symmetries in the computed eigenvalues. For the accuracy assessment of these computed eigenvalues, it is necessary to develop structured backward error analysis for structured eigenvalue problems. We undertake a detailed structured backward error analysis of a variety structured matrix pencils. We also discuss structured pseudospectra of these structured matrix pencils.

Verifying all eigen-pairs in real symmetric positive-definite generalized eigenvalue problem. **Shinya Miyajima** (Waseda University, Japan), Takeshi Ogita (Japan Science and Technology Agency), Shinichi Oishi (Waseda University, Japan) IC/CT2129/020

In this presentation, we are concerned with the accuracy of computed eigenpairs (eigenvalue λ and its corresponding eigenvector x) in the generalized eigenvalue problem

$$Ax = \lambda Bx$$

where A is a real symmetric matrix and B is a real symmetric positive definite matrix. The generalized eigenvalue problem widely appears in the field of scientific computing, e.g. stationary analysis of circuits, image processing, structure analysis and so forth. In many cases, it is known that A is real symmetric and B is real symmetric positive definite.
There are several methods for calculating guaranteed error bounds for approximate eigenvalues and eigenvectors. Among them, we consider in particular the case of verifying *all eigenpairs*. On verifying a few specified eigenvalues, see the papers by Behnke, Rump, Watanabe et al. and Yamamoto. On verifying a few specified eigenpairs, see the paper by Rump. On verifying all eigenvalues, see the paper by Maruyama et al..

On the other hand, the authors recently proposed a method of calculating guaranteed error bounds for all eigenpairs (μ, y) in the standard eigenvalue problem $Cy = \mu y$, where C is a real symmetric matrix.

In this presentation, we propose a fast method of verifying all eigenpairs for the generalized eigenvalue problem, which is an extension of the previous method by the authors. In the proposed method, intermediate results in the process of verifying all eigenvalues can be reused for verifying all eigenvectors. By this reuse, the computational cost for verifying all eigenvectors becomes almost negligible.

Our numerical results have confirmed that the proposed method supplies error bounds of sufficient quality. They have also confirmed that the computing time for the proposed method is almost the same as that for calculating all approximate eigenpairs.

Parameter analysis of the structure of regular matrix pencils by homotopic deviation theory. **Morad Ahmadnasab** (Universit Toulouse 1 and CERFACS, France) IC/CT1575/020

Let $A, E \in \mathbb{C}^{n\times n}$ be two given matrices, where $\operatorname{rank} E = r < n$. Matrix E is written in the form $E = UV^H$ where $U, V \in \mathbb{C}^{n\times r}$ have rank r. 0 is an eigenvalue of E with algebraic (resp. geometric) multiplicity m (resp. $g = n - r \le m$). We consider the regular pencil $P = (A - zI) + tE$, defined for $t \in \mathbb{C}$ and the parameter $z \in re(A) = \mathbb{C} \setminus \sigma(A)$, where $\sigma(A)$ denotes the spectrum of A.

We analyze how the structure [2] of the pencil P varies as $z \in re(A)$, by means of the notion of *frontier points*, which is essential in Homotopic Deviation theory [1]. At such points, $\operatorname{rank}(M_z) < r$, where $M_z = V^H(zI - A)^{-1}U$ is an $r \times r$ matrix defined for $z \in re(A)$.

When z is not (resp. is) a frontier point, the struture of the pencil P depends only on $r = \operatorname{rank} E$ but not on A (resp. depends on p_z, $1 \le p_z \le r$, the algebraic multiplicity of $0 \in \sigma(M_z)$). As an example, the structure of the regular pencil $A + tE$ when A is nonsingular and $z = 0$, is determined.

Work done in collaboration with Professor F. Chaitin-Chatelin.

[1] M. Ahmadnasab, F. Chaitin-Chatelin and N. Megrez; Homotopic Deviation in the light of Algebra. CERFACS Technical Report TR/PA/05/05 (2005).

[2] F. Gantmacher; *The theory of matrices*. Chelsea Publishing Company, New York, 1960.

Linear perturbation of structured matrix pencils arising in control theory. **Shreemayee Bora** (IIT Guwahati, India), Volker Mehrmann (TU Berlin, Germany) IC/CT2305/020

We develop a framework to analyse the effect of structure preserving linear perturbation on the eigenvalues of matrix pencils arising in linear quadratic optimal control and H_∞-control problems. The results complement and generalize some recent perturbation results for Hamiltonian matrices. The pencils (H, N), associated with the continuous and discrete time linear quadratic optimal control problems have Hamiltonian and symplectic spectral symmetry respectively and it is important to know the smallest structure preserving perturbation so that the perturbed pencil has eigenvalues on the imaginary axis in the former case and on the unit circle in the latter. We obtain necessary and sufficient conditions so that the perturbed pencils $(H + t\Delta H, N + t\Delta N)$, (where $t \in \mathbb{R}$, and ΔH and ΔN inherit the structures of H and N respectively) associated with the continuous time and discrete time versions of the problem have eigenvalues on the imaginary axis and the unit circle respectively. The second motivation is from the optimal H_∞-control problem where the recently developed process of γ-iteration (see [1] for references) involves computation of generalized Schur forms of two different one parameter families of pencils for the continuous and discrete time cases. We show that the parameter of smallest magnitude so that a corresponding pencil has purely imaginary eigenvalues in the continuous time case (respectively eigenvalues of unit modulus in the discrete time case) if it exists is the inverse of the largest real eigenvalue of a matrix much smaller than H or N.

[1] S. Bora and V. Mehrmann, Linear perturbation theory for structured matrix pencils arising in control theory. *SIAM J. Matrix Anal. Appl.,* Vol. 28(2006), No. 1, pp. 148 - 169.

A modified nodal approach to circuit synthesis. **Timo Reis** (TU Berlin, Germany) IC/CT4332/133

A popular result in analytic circuit theory is that for any positive real transfer function $G(s)$, an electrical circuit can be found whose impedance function is $G(s)$. We will reconsider the network realization problem from a differential-algebraic point of view. Given is a descriptor system

$$\begin{aligned} E\dot{x}(t) &= Ax(t) + Bu(t) \\ y(t) &= Cx(t) \end{aligned} \tag{1}$$

with a positive real $G(s) = C(sE - A)^{-1}B$. The aim is to perform state space transformations to (1) such that the resulting system is in modified nodal form, a structured differential-algebraic system arising in circuit modelling. From this form, an electrical circuit with the desired property can be directly constructed.

IC/CTS4597/02: Numerical methods for interpolation and approximation.

Organiser: Jean-Paul Berrut (Université de Fribourg, Switzerland)

Adjoint-based quasi-Newton methods for partially separable problems. **Sebastian Schlenkrich** (TU Dresden, Germany), Andrea Walther (TU Dresden, Germany) IC/CT1695/063

Partial separability was introduced by Griewank and Toint (1982) in the context of unconstrained optimization and nonlinear equations. It is based on the assumption that a function $F : \mathcal{R}^n \to \mathcal{R}^n$ can be represented as the sum of individual functions $F_j : \mathcal{R}^n \to \mathcal{R}^n$ for $j = 1 \dots k$. A quasi-Newton algorithm for solving $F(x) = 0$ may exploit the partitioning of F to approximate the Jacobian $F'(x)$ which is characterized by

$$F'(x) = \sum_{j=1}^{k} F'_j(x).$$

Thus sparsity or other structure of $F'(x)$ may be considered by the partitioning and the quasi-Newton method.

In this study the concepts of partitioned quasi-Newton methods are applied to Adjoint Tangent Rank-1 (ATR1) updates. ATR1 updates were introduced by Schlenkrich, Griewank, and Walther (2005). These updates have favorable properties for local and global convergence of the underlying quasi-Newton method. Consequently corresponding partitioned ATR1 updates are presented and local convergence results are established. Numerical results compare the partitioned ATR1 update methods to the corresponding unpartitioned quasi-Newton method and to Newton's method for nonlinear equations.

Direct discretization of the fractional-order differential by using Chebyshev series expansion. **Tsuyako Miyakoda** (Osaka University, Japan) IC/CT3270/021

We evaluate the fractional derivatives of some functions by applying the idea of a indefinite quadrature formula. To do this, we deal with the Chebyshev polynomial of the second kind to achieve the direct approximations to the fractional order(α)differential defined by

$$D^\alpha f(t) = \frac{d^m}{dt^m}\left[\frac{1}{\Gamma(m-\alpha)}\int_0^t \frac{f(r)}{(t-r)^{\alpha+1-m}}dr\right],$$

where $m - 1 < \alpha \le m, m \in N, \alpha \in R^+$. And we try to solve some fractional differential equations.

An hp finite-element method for singularly perturbed systems of reaction–diffusion equations. **Lisa Oberbroeckling** (Loyola College in Maryland, USA), Christos Xenophontos (University of Cyprus) IC/CT2351/021

We consider the approximation of a coupled system of two singularly perturbed linear reaction–diffusion equations, with the finite-element method. The solution to such problems contains boundary layers which overlap and interact and the numerical approximation must take this into account in order for the resulting scheme to converge uniformly with respect to the singular perturbation parameters.
We propose and analyze an hp finite element method which contains thin elements of size $O(p\varepsilon)$ and $O(p\mu)$ near the boundary, with ε and μ the singular perturbation parameters and p the degree of the approximating polynomials. We show that, under the assumption of analytic input data, the method converges at an exponential rate, as $p \to \infty$, independently of the singular perturbation parameters. Numerical results which validate the analysis and compare the proposed method with other schemes found in the literature will also be presented.

Pal-type interpolation on non-uniformly distributed points. **Hanuman Dikshit** (IIIT Jabalpur, India) IC/CT3443/015

Pal-type interpolation problems involving roots of unity and an additional point have been studied extensively. We have in (Numerical Algorithms, 40 (2005), 1-16) studied the regularity of certain Pal-type interpolation problems involving the $m-th$ roots of unity along with an additional point ζ and the $n-th$ roots of unity. We determine the largest domains for ζ, which ensure the regularity of the problems.

Numerical algorithm for a model of neuronal variability. **V.P. Ramesh Venkadachalam** (IIT Kanpur, India) IC/CT5063/021

In this, we analyse numerical approximation of a mathematical model of neuronal variabiliy by R.B. Stein. The model is in general a boundary value problem of singularly pertubed differential difference equation type with small shifts. Algorithm includes an appropriate approximation to the retarted arguments. A parameter uniform difference scheme is discussed. Test examples are solved to demonstrate the efficiency of the numerical scheme and also to show the effect of delays on the solution.

Some numerical methods for approximation of modified Bessel functions . **Juri Rappoport** (Russian Academy of Sciences) IC/CT733/021

Some numerical methods for the approximation of modified Bessel functions are described. The new realization of the Lanczos Tau method with minimal residue is proposed for the numerical solution of the second order differential equations with polynomial coefficients. The computational scheme of Tau method is extended for the systems of hypergeometric type differential equations. A Tau method computational scheme is applied to the approximate solution of a system of differential equations related to the differential equation of hypergeometric type. Various vector perturbations are discussed. The choice of the perurbation term in the form of a shifted Chebyshev polynomial with a special kind of selected transition and normalization is suggested. The minimality conditions for the perturbation term are found for one equation. They are sufficiently simple for the verification in a number of important cases. Several approaches for the computation of kernels of Kontorovitch-Lebedev integral transforms - modified Bessel functions of the second kind with pure imaginary and complex order are elaborated. The codes of the evaluation are constructed and tables of the modified Bessel functions are published. The comparisons are discussed. The advantages of suggested algorithms and codes in accuracy and timing are shown. The effective applications for the numerical solution of some mixed boundary value problems in wedge domains are given.

IC/CTS4613/02: Numerical methods for interpolation and approximation.

Organiser: Jean-Paul Berrut (Université de Fribourg, Switzerland)

First applications of a formula for the error of finite sinc-interpolation. **Jean-Paul Berrut** (Université de Fribourg, Switzerland) IC/CT2171/021

We consider the interpolation of a function $f \in C^{2m+2}(\mathbb{R})$ between the equidistant abscissae $x_n = nh$, $h > 0$, $n \in \mathbb{Z}$. Sinc-interpolation is based on a dilation and a series of shifts of the *sinus-cardinalis* function $\mathrm{sinc}(x) := \sin(x)/x$. It often converges very rapidly, so for example for functions analytic in an open strip containing the real line and which decay fast enough at infinity. This decay does not need to be very rapid, however, as in Runge's function $1/(1+x^2)$. Then one must truncate the series, and this truncation error is much larger than the discretisation error (it decreases algebraically as opposed to exponentially for the latter). In 2003 we have discovered a formula for the error $C_N(f,h) - f$ of the truncated series

$$C_N(f,h)(x) := \sum_{n=-N}^{N}{}'' \mathrm{sinc}\left[\frac{\pi}{h}(x-x_n)\right] f_n, \qquad h = \frac{X}{N},$$

for an approximation on the interval $[-X,X]$, where the double-prime means that the first and last terms are halved. The formula reads

$$C_N(f,h)(x) = f(x) + \frac{(-1)^N}{2\pi} \sin\frac{\pi}{h}x \sum_{k=1}^{m} a_{2k}(x)(2h)^{2k} + \mathcal{O}(h^{2m+2}),$$

with

$$a_{2k}(x) := 2(1-2^{-2k})\frac{B_{2k}}{(2k)!}\left[\left(\frac{f(y)}{x-y}\right)^{(2k-1)}(X) - \left(\frac{f(y)}{x-y}\right)^{(2k-1)}(-X)\right]$$

and where the B_k denote the Bernoulli numbers.
In our talk we shall give first applications of the formula, such as its use for correcting $C_N(f,h)$ with derivatives and finite differences, elimination of the Gibbs phenomenon, extrapolation to the limit, the barycentric formula, an error formula for one-sided sinc-interpolation, also.

Nonlocal-means single-frame image zooming. **Mehran Ebrahimi** (University of Waterloo, Canada), Edward Vrscay (University of Waterloo, Canada) IC/CT3505/021

We present a novel single-frame image zooming that combines the ideas of fractal-based image zooming, example-based zooming, and nonlocal-means image denoising in a consistent and improved framework.

The idea of increasing the resolution of an image using its nonlocal self-similarities was initially proposed by the researchers in fractal image coding back in the 1990s. In fractal image coding, one seeks to approximate a target image by the fixed point of a contractive, resolution-independent operator called the fractal transform.

A more recent series of novel example-based methods that take advantage of the self-similarity of images show great promise for the solution of various inverse problems. In 2005, A. Buades et al., demonstrated that their nonlocal-means (henceforth to be referred to as "NL-means") image denoising algorithm has the ability to outperform classical denoising

methods. In this paper, we generalize their method to address the zooming problem.

Similar to NL-means denoising, we compare neighborhoods in the image to predict pixel intensities. Our algorithm compares the neighborhood information of each pixel to the neighborhoods of the same size in the coarser scale over the entire image.

In Bayesian terms, our zooming technique targets the MMSE estimate by learning the posterior directly from examples taken from the image itself at a different scale, similar to fractal-based techniques.

We will address various computational issues and various results of this zooming technique applied to natural images will be presented. Due to the reconstruction scheme, our results do not suffer from the blockiness generally inherent in fractal zooming. Moreover, the geometry of objects is well preserved for the test images presented.

Learning multiresolution schemes for compression of images. **Dionisio Yanez** (Universitat de València, Spain), Paco Arandiga (Universitat de València, Spain), Albert Cohen (Université Paris VI, France) IC/CT3078/021

Learning theory plays a key role in the several scientific fields such as statistics, data mining, artificial intelligence, as well as in some engineering areas. Multiscale decompositions are a well stablished tool that aims at a rearrangement of the information contents in a set of discrete data. Multiresolution transform are based on transfer operators connecting consecutive resolution levels. In this work we apply learning techniques in order to construct one of the key operators of multiscale decompositions within Harten's multiresolution framework: the prediction operator. When applied to the compression of images, 'Learning' can be used to obtain nearly-optimal filters for the prediction process for images on a given library or class. We perform several numerical experiments with these newly designed "learning-multiresolution" transforms and compare our results with the results obtained with other more classical methods.

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[4] Vladimir N. Vapnik; The Nature of Satitstical Learning Theory. *Springer* 1995.

Exact asymptotics of the uniform error of interpolation by multilinear splines. **Yuliya Babenko** (Sam Houston State University, USA) IC/CT4293/021

In this talk we will investigate the questions of adaptive approximation of C^2 functions by multilinear splines. In particular, we will provide the exact formula to describe the asymptotic behavior of the optimal error of the weighted uniform approximation by interpolating and quasi interpolating splines from this class.

Quasi-interpolation based on bivariate C^1 quadratic B-splines with multiple knots. **Paola Lamberti** (Università degli Studi di Torino, Italy), Catterina Dagnino (Università degli Studi di Torino, Italy), Sara Remogna (Università degli Studi di Torino, Italy) IC/CT1698/021

Taking into account the results[1,2,3] on bivariate spline quasi-interpolation and on the effects of multiple knots[4], in this paper we define, analyse and generate local quadratic spline quasi-interpolants on criss-cross triangulations of a rectangular domain Ω, with possible multiple knots inside Ω and/or on the boundary $\partial\Omega$. Such splines can be particularly useful in mechanics and engineering applications, since they can model constrained surfaces with different kind of smoothness in Ω. A computational procedure for their construction is proposed and some applications with numerical and graphical results are presented.

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[2] C. Dagnino, P. Sablonnière; Error analysis for quadratic spline quasi-interpolants on non-uniform criss-cross triangulations of bounded rectangular domains. Prépublication IRMAR 06-06 (2006).

[3] P. Sablonnière; On some multivariate quadratic spline quasi-interpolants on bounded domains. In: Modern developments in multivariate approximations (Eds. W. Hausmann & al.), ISNM Vol. 145, Birkhauser Verlag, Basel (2003), 263–278.

[4] R.-H. Wang, C.-J. Li; A kind of multivariate NURBS surfaces. J. Comp. Math. 22, no. 1 (2004), 137–144.

On Blackman–Harris windows for Shannon sampling series. **Gert Tamberg** (Tallinn University of Technology, Estonia) IC/CT2623/021

A Shannon sampling series is a representation of a function as a function series with its samples as the expansion coefficients. Using different kernels we get generalized sampling series, widely studied at RWTH Aachen since 1977[1]. Sampling theory obeys applications in several disciplines where functions have to be reconstituted from measurements or sampled data. In image processing sampling series give us a natural way to perform operations on images, seen as continuous functions.

In this presentation we consider approximations by the sampling series $C_{W,\mathbf{a}}f$, which are defined by the Blackman–Harris (or cosine-sum) window functions (the Blackman window has been used in signal analysis over 40 years). The choice of parameters $\mathbf{a}$ in Blackman–Harris window allows us to get kernels, suitable for different applications[2,3,4].

We estimate the order of approximation $\|f - C_{W,\mathbf{a}}f\|$ via the modulus of continuity. In the case of certain (m+1)-term cosine-sum window functions the order of approximation can be estimated via the $2m$-th modulus of continuity.

We give also different type of upper and lower bounds for the operator norms of $C_{W,\mathbf{a}} : C(\mathbb{R}) \to C(\mathbb{R})$.

[1] P.L. Butzer, G. Schmeisser and R.L. Stens; An introduction to sampling analysis. In: *Nonuniform Sampling, Theory and Practice* (F. Marvasti, ed.), Kluwer/Plenum, 2001, pp.17–121

[2] A. Kivinukk and G. Tamberg; Blackman-type windows for sampling series. J. of Comp. Analysis and Applications, **7** (2005), pp.361–372.

[3] A. Kivinukk, G. Tamberg; On Blackman–Harris windows for Shannon sampling series. Sampling Theory in Signal and Image Processing (accepted).

[4] G. Tamberg; Approximation by the Blackman-type sampling series. In: *Proc. of the Intern. Workshop on Sampling Theory and Applications (SampTA'03), Strobl, Salzburg, Austria, May 26–31, 2003*, pp.9-0-94.

IC/CTS4592/02: **Numerical methods for integral equations.**

Organiser: Per-Gunnar Martinsson (University of Colorado at Boulder, USA)

Solutions of Volterra integro-differential equations with rapidly vanishing convolution kernels. **Barbara Zubik-Kowal** (Boise State University, USA), Zdzislaw Jackiewicz (Arizona State University, USA), Frank Hoppensteadt (New York University, USA) IC/CT18/023

Nonlinear systems of Volterra integro-differential equations (VIDEs) of convolution type are studied. Important examples of such problems which motivate our investigations are VIDEs, which model the thalamo-cortical systems describing a new architecture for a neurocomputer.

Such a neurocomputer is modelled in [1] and [2]. The model employs principles of the human brain and is described using systems of VIDEs. Since such a neurocomputer consists of many interconnected units (referred as neurons), the thalamo-cortical systems include large numbers of VIDEs. Therefore, robust and efficient numerical algorithms are needed for computer simulations for the solutions to the systems.

In this presentation, we propose an iteration technique to solve the thalamo-cortical systems numerically. The proposed successive iterates are vector functions of time, which change the original problems into systems of separated equations. Such separated equations can then be solved in parallel computing environments.

We analyze the convergence of the successive iterates by using the properties of the kernels of the thalamo-cortical models. Our theoretical results are confirmed by numerical experiments.

[1] F. C. Hoppensteadt and E. M. Izhikevich; *Oscillatory Neurocomputers with Dynamic Connectivity*. Phys. Rev. Lett. **82** (1999), 2983–2986.

[2] Y. Kuramoto; *Chemical Oscillations, Waves, and Turbulence*. Springer-Verlag, New York, 1984.

Numerical methods for 2D weakly-singular Volterra integral equations of the second kind. **Alexander Tynda** (Penza State University, Russian Federation) IC/CT723/023

The talk is dedicated to the numerical solution of two-dimensional Volterra weakly-singular integral equations of the form

$$x(t_1,t_2) - \int_0^{t_2}\int_0^{t_1} H(t_1,t_2,s_1,s_2)x(s_1,s_2)ds_1ds_2 = f(t_1,t_2),$$
$$(t_1,t_2) \in D = \{(t_1,t_2) : 0 \le t_1,t_2 \le T,\}$$

which kernels $H(t_1,t_2,s_1,s_2)$ may have two kinds of singularities:

$$H = \frac{h(t_1,t_2,s_1,s_2)}{\left((t_1-s_1)^2+(t_2-s_2)^2\right)^{\alpha}} \qquad H = \frac{h(t_1,t_2,s_1,s_2)}{(t_1-s_1)^{\alpha_1}(t_2-s_2)^{\alpha_2}}.$$

We assume that h and f have continuous derivatives up to certain order $m+1$; $0 < \alpha, \alpha_1, \alpha_2 < 1$.

In order to weaken the singularity influence on the numerical computation we transform the equation in both cases into equivalent equation. The piecewise polynomial approximation of the exact solution is then applied. For numerical computing of the nascent weakly singular integrals we construct the special Gauss-type cubature formula based on nonuniform grid.

Also we suggest the practical mesh which is less nonuniform than standard graded mesh $t_k = \left(\frac{k}{N}\right)^{r/(1-\alpha)} T$, but at the same time it gives us an equivalent approximation error for the functions from $C^{r,\alpha}(0,T]$.

Economical discretization schemes in the finite-section method. **Evgeniya Lebedeva** (Ukraine, Kiev), Sergei Solodky (Institute of Mathematics, Kiev, Ukraine) IC/CT1516/023

Consider a first-kind Fredholm integral equation

$$Az(t) := \int_0^{\infty} k(t,\tau)b(\tau)(1+\tau)^{-s/2}z(\tau)d\tau = y(t). \quad (1)$$

where $z(t), y(t) \in L_2(0,\infty)$, $k(t,\tau), b(\tau) \in C(0,\infty)$ and $|k(t,\tau)| \le c_k[(1+t)(1+\tau)]^{-\kappa}$, $|b(\tau)| \le c_b\tau^{\beta}$, $\kappa > 1/2$, $s > 2\beta - 2\kappa + 1$. Suppose that $y_\delta(t) \in L_2(0,\infty)$ is known instead of $y(t)$ and $\|y - y_\delta\|_{L_2(0,\infty)} \le \delta$. Let $a(t,\tau) := k(t,\tau)b(\tau)(1+\tau)^{-s/2}$ satisfies the conditions $|a^{(i,j)}(t,\tau)| \le c(1+t)^{-\alpha}(1+\tau)^{-\omega}, i,j = 0,1$ at some $\alpha,\omega > 1/2$. Many inverse problems in optic and astronomy are described by the equation (1) (see [1]).

Let P_M be an orthoprojector from $L_2(0,\infty)$ to $L_2(0,M)$. According to finite-section method we pass from (1) to the equation

$$P_{2^n}AP_{2^m}z(t) := \int_0^{2^m} a(t,\tau)z(\tau)d\tau = P_{2^n}y_\delta(t), t \in [0,2^n),$$

Consider the system of knots $t^{\theta}_{0,q,i} = i2^{-q}$, $t^{\theta}_{k,q,i} = 2^{k-1} + i2^{k-1}M^{-1}_{k,\theta}$, $k = 1,2,3,...,i = 0,1,...M_{k,\theta}$, $M_{k,\theta} = [2^{k(1-\theta)+q}]$. Here $0 < \theta \le 1$ and $q \in N$ are some fixed numbers, $[u]$ is integer part of u. Let's construct a function interpolating $a(t,\tau)$ at the points of grid above:

$$S^q_{k,l}(a;t,\tau) = \sum_{i=1}^{M_{k,\theta_1}}\sum_{j=1}^{M_{l,\theta_2}} a(t^{\theta_1}_{k,q,i-1}, \tau^{\theta_2}_{l,q,j-1})S_{k,i}(t)S_{l,j}(\tau), \quad (2)$$

where $S_{k,i}, S_{l,j}$ are characteristic functions of the intervals $[t^{\theta_1}_{k,q,i-1}, t^{\theta_1}_{k,q,i})$ and $[t^{\theta_2}_{l,q,j-1}, t^{\theta_2}_{l,q,j})$. Denote the total volume of values for $a(t^{\theta_1}_{k,q,i}, \tau^{\theta_2}_{l,q,j})$ as Card. A scheme with smaller quantity of Card is called more economical. As is well known, for achievement of order-optimal error it is necessary to approximate $P_{2^n}AP_{2^m}$ with accuracy $O(\delta)$.

Statement of problem. It is required to construct economical discretization scheme of operator $P_{2^n}AP_{2^m}$ so that the kernel of finite-dimensional operator A' is a sum of functions (2) and $\|A' - P_{2^n}AP_{2^m}\| = O(\delta)$.

Suppose $\mu = \kappa - 1/2$, $\lambda = \kappa + \frac{s}{2} - \beta - \frac{1}{2}$, Let $\mu > \lambda$, then at $m > n$ we fix $\forall d \in R : 1 < d < \min\{\frac{\mu}{\lambda}, \frac{m}{n}\}$. Let's construct the kernel of operator A' as $\sum_{k=1}^{n}\sum_{l=1}^{m-dk} S^q_{k,l}(a;t,\tau) + \sum_{k=1}^{n} S^q_{k,0}(a;t,\tau) + \sum_{l=1}^{m} S^q_{0,l}(a;t,\tau) + S^q_{0,0}(a;t,\tau)$.

Theorem. *If m,n,q are such that $2^m \asymp \delta^{-\frac{1}{\lambda}}, 2^n \asymp \delta^{-\frac{1}{\mu}}, 2^q \asymp \delta^{-1}\sqrt{\log(1/\delta)}$, then A' satisfies condition above and order bounds for* Card *hold true a) $\delta^{-2}\log^3\frac{1}{\delta}$, if $\theta_1 = \theta_2 = 1$; b) $\delta^{-2-\frac{1-\theta_1}{\mu}}\log^2\frac{1}{\delta}$, if $\theta_1 < 1$, $\theta_2 = 1$ or $\theta_1 < \theta_2 < 1$, $d = \frac{1-\theta_1}{1-\theta_2}$; c) $\delta^{-2-\frac{1-\theta_2}{\lambda}}\log\frac{1}{\delta}$, if $\theta_1 = 1$, $\theta_2 < 1$ or $\theta_1 < \theta_2 < 1$, $d > \frac{1-\theta_1}{1-\theta_2}$ or $\theta_2 < \theta_1 < 1$ or $\theta_1 = \theta_2 < 1$; d) $\delta^{-2-\frac{1-\theta_2}{\lambda}-\frac{1-\theta_1-d(1-\theta_2)}{\mu}}\log\frac{1}{\delta}$, if $\theta_1 < \theta_2 < 1$, $d < \frac{1-\theta_1}{1-\theta_2}$.*

At $\theta_1 + \theta_2 < 2$ proposed scheme is more economical as compared to standard one[1]. For $\lambda \ge \mu$ new economical discretization schemes have also been constructed.

[1] Pereverzev, S. and Schock E.; The finite-section approximation for ill-posed integral equations on the half-line. J. Integral Equations Appl. 11 (2001), pp.501–513.

A fast algorithm for the inversion of boundary integral operators. **Per-Gunnar Martinsson** (University of Colorado at Boulder, USA) IC/CT3211/023

In this talk, we will present a fast algorithm that directly constructs a compressed representation of the inverse of an integral operator. When applied to boundary integral equations in two dimensions involving non-oscillatory or moderately oscillatory kernels, the computational complexity of the scheme is $O(N)$, where N is the number of degrees of freedom in the discretization.

Through several computational examples, we will demonstrate that the algorithm can effectively solve integral equations that are not well-suited for iterative solvers, such as scattering problems involving cavities. We will also show that for problems involving multiple right-hand-sides, the scheme is between one and two orders of magnitude faster than iterative solvers based on the Fast Multipole Method.

A generalization to an algorithm for inverting boundary integral operators in three dimensions will be discussed, as well as methods for rapidly computing spectral decompositions of integral operators. Furthermore, comparisons will be made with similar schemes that have been published by other authors in the last ten years.

Work done in collaboration with Vladimir Rokhlin and Mark Tygert.

IC/CTS4600/02: Numerical methods for ODEs and DAEs.

Organiser: John Butcher (University of Auckland, New Zealand)
Co-organiser: Juan Ignacio Montijano (Universidad de Zaragoza, Spain)

Order stars and order arrows. **John Butcher** (University of Auckland, New Zealand) IC/CT3375/024

The use of order stars in the analysis of stability questions is well-known. In particular, the Ehle barrier was first proved using this approach. This and related results can sometimes also be proved using "Order arrows" and a survey of this alternative technique will be presented. Given a sequence of integers $[n_0, n_1, \ldots, n_r]$, a generalized Padé approximation to the exponential fiunction is a sequence of polynomials $(P_0, P_1, \ldots, P_r)$ such that $\sum_{i=0}^{r} \exp((r-i)z)P_i(z) = O(z^{p+1})$, where the order p is equal to $\sum_{i=0}^{r}(n_i+1)-1$. Using a definition of A-stability related to the application of these approximations to multivalue methods for the solution of initial value poblems, it was conjectured by F. Chipman and the author that $2n_0 \le p+2$ is a necessary condition. In the case $r=1$, this is the Ehle barrier. A proof of the general case $r \ge 1$ will be presented.

The reliability/efficiency trade-off for a new class of ODE solvers. **Wayne Enright** (University of Toronto, Canada) IC/CT2433/024

In the numerical solution of ODEs, it is now possible to develop efficient techniques that will deliver approximate solutions that are piecewise polynomials. The resulting methods can be designed so that the piecewise polynomial will satisfy a perturbed ODE with an associated defect (or residual) that is directly controlled in a consistent fashion. We will discuss the reliability/efficiency trade off that one faces when implementing and using such methods. In particular we will identify a new class of continuous Runge–Kutta methods with a reliable defect estimator and a validity check that reflects the credibility of the estimate.

Numerical results on a wide selection of problems will be summarised for methods of orders four through eight. It will be shown that a modest increase in the cost per step can lead to a significant improvement in the robustness and reliability of the method.

Convergence of the generalized-α method applied to differential-algebraic equations of index 3 . **Martin Arnold** (Universität Halle–Wittenberg, Germany) IC/CT3364/024

The generalized-α method belongs to the class of Newmark type methods that are frequently used for the time integration of finite element models in structural dynamics. Recently, these methods have also been applied successfully in multibody dynamics to solve numerically the equations of motion of constrained mechanical systems.

In the present paper, the application of the generalized-α method to a class of second order differential-algebraic equations of index 3 is considered in more detail (see also M. Arnold, O. Brüls: *Convergence of the generalized-α scheme for constrained mechanical systems.* - accepted for publication in: Multibody System Dynamics, 2007). Convergence is analysed using an equivalent multistep representation of the method. Second-order convergence is demonstrated for all solution components including the algebraic ones.

From a practical viewpoint, the application of these results to the index-3 formulation of the equations of motion for constrained mechanical systems is of particular interest. Numerical tests for a benchmark problem illustrate practical implications of the convergence analysis.

Analysis of a multirate θ-method for stiff ODEs. **Valeriu Savcenco** (CWI, Amsterdam, The Netherlands) IC/CT4565/024

To solve ODE systems with different time scales which are localized over the components, multirate time stepping can be used. We present a study of a simple multirate scheme, consisting of the θ-method with one level of temporal local refinement. Issues of interest are local accuracy, propagation of interpolation errors and stability. The theoretical results are illustrated by numerical experiments, including results for more levels of refinement with automatic partitioning.

Dynamic optimization and nonlinear differential–algebraic equations in computational chemistry. **Alexandre Caboussat** (University of Houston, USA), Jiwen He (University of Houston, Switzerland), Chantal Landry (École Polytechnique Fédérale de Lausanne, Switzerland) IC/CT2448/024

Dynamic optimization problems arise when coupling an optimization problem with ordinary differential equations. This problem appears for instance in computational chemistry when a system at equilibrium exchanges mass with a surrounding media. A stiff system of differential-algebraic equations is obtained when replacing the optimization problem with its first order optimality conditions.

In this talk, we discuss numerical methods for the efficient resolution of a system of differential-algebraic equations arising in the modeling of the dynamics of atmospheric organic aerosol particles. The minimization of the Gibbs free energy with equality and inequality constraints is coupled with differential equations when the constraints of the optimization problem depend on time.

The static minimization problem consists in computing the convex envelope of the energy. We propose a primal-dual interior-point method for the determination of this global optimum and introduce the notion of phase simplex related to

the convex envelope to describe mathematically the optimum. We solve the Karush-Kuhn-Tucker system of nonlinear equations that consists of the first order optimality conditions. Efficient numerical linear algebra methods, using Schur complement and null-space methods, are designed for the resolution of the resulting Newton system.

We extend the methodology to the time-variable optimization problem arising when the optimization problem is coupled with differential equations. The first order conditions, together with an implicit discretization of the differential equations, form an extended system that is solved with sequential quadratic programming techniques, by controlling the inertia of the linear system. The detection of discontinuities in the trajectories, due to the inequality constraints in the optimization problem, are discussed. Numerical results are presented for the computation of the thermodynamic equilibrium and mass transfer of organic aerosols.

A note on the error growth in the numerical integration of periodic orbits. **Juan Ignacio Montijano** (Universidad de Zaragoza, Spain), Manuel Calvo-Pinilla (Universidad de Zaragoza, Spain), Pilar Laburta (Universidad de Zaragoza, Spain), Luis Rández (Universidad de Zaragoza, Spain) IC/CT4068/024

Periodic and small perturbations of periodic solutions appear frequently associated to systems of differential equations in many applications. There has been a considerable amount of work investigating how numerical integrators perform on periodic orbits, in particular in the long-time integration. Thus B. Cano and J. M. Sanz-Serna (SIAM J. Numer. Anal. , 1997) analyze the growth of the global error in the numerical integration with one-step methods of such class of problems, with special attention to Hamiltonian and reversible systems.

The aim of this work is to extend this analysis in two ways. On one side considering systems with a periodic solution embedded into a family of periodic orbits. More precisely, for each $\hat{x}$ in a neighborhood of the initial condition x_0, the solution of $x' = f(x)$, $x(0) = \hat{x}$ is also periodic with period $T = T(x)$ where the function T is as smooth as required. For this class of problems we show that the monodromy matrix of $x(t)$ can be expressed in terms of the gradient $\nabla T(x_0)$ and that the global error after N periods $ge^{(N)}$ is affected by a linear term $Nge^{(1)}$ and a quadratic term in N whose coefficient depends on $\nabla(x)^T ge^{(1)}$. It is shown that if the period depends only on some invariants of the problem and the numerical method preserves these invariants, the global error behaves as $\mathcal{O}(N)$. On the other hand we study the behavior of the error in the invariants when a problem with some conservation property and periodic solution is integrated. We show that for most one-step methods the invariant error behaves as $\mathcal{O}(N)$.

IC/CTS4602/02: Numerical methods for ODEs and DAEs.

Organiser: Roger Sidje (University of Queensland, Australia)

Computation of the Mittag-Leffer matrix function that arises in fractional differential equations. **Roger Sidje** (University of Queensland, Australia) IC/CT4803/024

Although not as widely known as other special functions, the Mittag-Leffer function, which is a generalization of the exponential function, is gaining prominence owing to its usefulness when modelling certain physical and biological processes with anomalous diffusion. Such processes are formulated in terms of derivatives (and integrals) of fractional (non-integer) order. Of particular interest is the development of numerical methods for computing the Mittag-Leffer function, especially in the case where its argument is a matrix of potentially large dimension. We discuss Krylov subspace techniques and related issues to address this problem.

On collocation method by orthogonal 0-interpolants. **Muhammad Bokhari** (King Fahd University, Saudi Arabia), Hussain Al-Attas (King Fahd University, Saudi Arabia) IC/CT3510/024

Most of the engineering and scientific problems give rise to boundary value problems for which the method of finding analytic solution is either very complicated or sometimes impossible. The collocation methods are widely used to determine approximate solution of such problems. Among these the orthogonal collocation method is quite prominent. This method leads to fourth order convergence. Recently, we have introduced the notion of orthogonal 0-interpolants and applied it to determine certain constrained approximation problems. These interpolants have free zeros like the standard orthogonal polynomials and also some pre-assigned zeros. Here, we discuss a collocation method based on a combination of fixed and free zeros of orthogonal 0-interpolants. We shall present an outcome of comparative study of our suggested method with the standard orthogonal collocation method.

Absolutely-stable explicit schemes for reaction systems. **Chang-Ock Lee** (KAIST, Republic of Korea), Eun-Hee Park (KAIST, Republic of Korea), Jae Boum Youm (Inje University, Republic of Korea), Chae Hun Leem (University of Ulsan, Republic of Korea) IC/CT2859/024

Many phenomena of interest in physiology and biochemistry are characterized by reactions among several chemical species and diffusion in various mediums. In a closed system, both reactions and diffusion are governed by a system of ordinary differential equations (ODEs)

$$\dot{\mathbf{y}}(t) = M\mathbf{y}(t), \tag{1}$$

which guarantees conservation of the total amount of $\mathbf{y}(t)$ for any $t \geq 0$. Since we are concerned with the steady-state solution as well as the transient in simulations of very large systems of chemical reactions or molecular dynamics, we need to take the overall computational cost into consideration. Many physiologists and biochemists prefer explicit methods to implicit methods since implementation of the explicit methods is easier than the others. The popular methods for reaction systems are simple explicit schemes such as Euler's method, Runge-Kutta method, etc. However, it is well-known that conditional stability, the typical weak point of explicit methods, is very fatal for stiff problems. In the past few decades, many studies on numerical methods for stiff ODEs have been done in various aspects.

The aim of this talk is to present two absolutely stable explicit schemes which are applicable to a general reaction system (1). The proposed methods are motivated by the simple exact solver for a reversible reaction. In spite of their explicitness, we have unconditional stability, that is, stability without any condition on the step size. Furthermore, we proved the convergence of the proposed methods; one is of first order and the other is of second order.

Adaptive τ method for ODEs. **Seyed Mohammad Hosseini** (Tarbiat Modares University, Iran) IC/CT198/024

The Tau method for solving differential equations has been the topic of research in last 30 years. For ordinary differential equations over long intervals and particularly for stiff equations it requires very small step lengths and so it is not generally successful. We introduce an adaptive strategy with which this method can solve stiff odes efficiently. In this work we discuss and compare different merits of variable and fixed time step Tau method.

Numerical solution of fractional differential, integral and integro-differential equations by using piecewise-constant orthogonal functions. **Ali Salimi Shamloo** (Islamic Azad University of Shabestar, Iran), Esmaeil Babolian (Tarbiat Moallem University, Iran) IC/CT4339/002

In this paper, we use operational matrices of piecewise constant orthogonal functions on the interval $[0,1]$ to solve fractional differential, integral and integro-differential equations. We first use operational matrices and then convert the problem to a system of linear equations. Numerical examples show that the approximate solutions have a good degree of accuracy.

Keywords: Fractional differential equations, Fractional integral equations,Fractional integro-differential equations, Piecewise constant orthogonal functions, Operational matrices.

Numerical solution of the system of Fredholm integro-differential equations by the τ method. **Jafar Pourmahmoud Gazijahani** (Azarbijan University of Tarbiat, Iran), Sedghat Shahmorad (University of Tabriz, Iran) IC/CT664/023

The τ method, produces approximate polynomial solution of differential, integral and integro-differential equations (see [E.l,Ortiz, The Tau method, SIAM J. Numer. Anal. 6 (3) (1969) 480Ű492; E.l. Ortiz, H. Samara, An operational approach to the Tau method for the numerical solution of non-linear differential equations, Computing 27 (1981) 15Ű25; S.M. Hosseini, S. Shahmorad, A matrix formulation of the Tau for Fredholm and Volterra linear integro-differential equations, The Korean J. Comput. Appl. Math. 9 (2) (2002) 497Ű507; S.M. Hosseini, S. Shahmorad, Numerical solution of a class of integro-differential equations by the Tau method with an error estimation, Appl. Math. Comput. 136 (2003) 559Ű570]). In this paper, we extend the Tau method for the numerical solution of integro-differential equations systems (IDES). We also give a brief description of the structure of the Tau program by the Maple software. An efficient error estimation of the numerical solution of the method is also introduced. Some examples are given to clarify the efficiency and high accuracy of the method.

Keywords: Operational Tau method; Integro-differential equations

IC/CTS4618/02: Numerical methods for PDEs: evolution problems.

Organiser: Christina Christara (University of Toronto, Canada)

On the free-boundary formulation for parabolic problems. **Salvatore Iacono** (Università degli Studi di Messina, Italy), Riccardo Fazio (Università degli Studi di Messina, Italy) IC/CT3997/025

The aim of this paper is to propose an original numerical approach for parabolic problems whose governing equation are defined on an infinite domain. We are interested in analysing the class of problems admitting invariance property to Lie group of scalings. Thanks to similarity analysis, in such a way the parabolic problem can be transformed to an equivalent boundary value problem governed by an ordinary differential equation and defined on an infinite interval. A free boundary formulation and a convergence theorem for this kind of transformed problems are available in [Fazio, SIAM J. Numer. Anal., 33 (1996), pp. 1473-1484]. Depending on its scaling invariance properties, the free boundary problem is then solved numerically using either an iterative or non-iterative method. Finally, the solution of the parabolic problem is retrieved applying the inverse map of similarity.

Finite-element method for semilinear parabolic interface problems. **Rajen Sinha** (IIT Guwahati, India) IC/CT238/025

We study the convergence of finite element solution to the exact solution of a semilinear parabolic interface problem in a two dimensional convex polygonal domain. If the triangulation is isoparametrically fitted to the interface then optimal order error estimate is achieved in $L^2(H^1)$-norm for the semidiscrete scheme. Based on backward Euler method, a fully discrete scheme is also analyzed and the related convergence result is established. The interface is assumed to be of arbitrary shape and is smooth for our purpose.

Flux-based level-set method: a finite-volume method for evolving interfaces. **Christian Wehner** (Universität Heidelberg, Germany) IC/CT3665/025

The flux-based level-set method is a finite volume method for solving hyperbolic equations arising in the level-set formulation of interface evolution. The motion can be defined by an external velocity field or by a velocity depending on the normal direction of the interface. The method is second-order accurate for smooth solutions and shows good behaviour in more involved cases like deformation flow fields or expanding square.

Several applications will be presented, including the modeling of convection-diffusion in two-phase flow, reinitialization of the level-set function an the problem of sail-boat distances. The simulations are realized using Matlab.

Spline collocation for parabolic partial differential equations. **Christina Christara** (University of Toronto, Canada) IC/CT3146/025

Collocation is a simple to implement discretization technique for differential equations' problems that gives an approximation to the solution over the whole domain of the problem. Spline collocation has been primarily used for the solution of Boundary Value Problems for ODEs or PDEs, and shown to be an effective method. Two types of spline collocation methods have been developed, the extrapolated (a.k.a. modified) and the deferred-correction methods, both giving rise to optimal order of convergence to the solution. These methods have been extended recently to non-uniform grids and integrated with adaptive techniques. In this presentation, we are concerned with spline collocation methods for parabolic PDEs. In particular, we consider quadratic and cubic spline collocation formulated as deferred-correction methods and combined with finite difference time discretization techniques. Deferred-correction methods normally require the solution of two linear systems per timestep. We discuss ways to avoid the solution of the second linear system, thus improving the efficiency of the methods, without sacrificing accuracy and stability. We also present the difficulties to incorporate adaptive techniques in the space dimension(s), while maintaining the efficient formulation of the methods and suggest ways to overcome them.

Adaptive techniques for parabolic problems using deal.II software. **Nupur Gupta** (IIT Bombay, India), Neela Nataraj (IIT Bombay, India), Andreas Griewank (Humboldt-Universität zu Berlin, Germany) IC/CT3639/025

The work is based on finding error control and adaptive mesh designing for evolution problems in 2 dimensions. For numerical results the software deal is being used and memory consumption issue is also discussed. Error estimators are also being calculated using duality argument as in priori error estimates.

Numerical propagator method solutions for the linear parabolic initial boundary-value problems. **Janis Rimshans** (Latvijas Universitate, Latvia), Sharif Guseynov (Latvijas Universitate, Latvia) IC/CT3029/025

Solubility of the linear initial-boundary value problem containing lower order derivatives is discussed. Initial-boundary value problem is formulated as follows:

$$\partial_t C = \nabla \cdot D\nabla C + f(\nabla C, C, t, x), \qquad in \quad \Omega, \tag{1}$$

$$D\nabla C \cdot \nu + \gamma C = \vartheta(t), \qquad on \quad \partial\Omega, \tag{2}$$

$$C(0,x) = C_0(x), \tag{3}$$

where D is bounded and positive defined, γ and ϑ are given functions.

By using Green function approach analytical solution consistent with solubility conditions of the problem is formulated for the case of constant coefficients of parabolic equation. On the base of numerical propagator method a new finite volume difference scheme is proposed. Stability of the scheme is investigated taking in to account obtained analytical solutions of the initial-boundary value problem $(1)--(3)$. Numerical tests are presented.

IC/CTS4632/02: Numerical methods for PDEs: evolution problems.

Organiser: Prabir Daripa (Texas A&M University, USA)
Co-organiser: Quang Long Nguyen (Institut Français du Pétrole, France)

Lagrange-projection scheme for two-phase flows: 1. application to realistic test cases. **Quang Long Nguyen** (Institut Français du Pétrole, France), Frederic Coquel (Université Pierre et Marie Curie, France), Marie Postel (Université Pierre et Marie Curie, France), Quang Huy Tran (Institut Français du Pétrole, France) IC/CT2286/025

We are concerned with the numerical simulation of two-phase flows representing oil transportation along a 1-D pipeline. More specifically, we wish to show that, for this kind of problems, it is highly recommended to make use of the Lagrange-Euler projection formalism. Indeed, this approach naturally splits the effects of slow (kinematic) and fast (acoustic) waves, thus enabling us to design a numerical scheme with several desirable properties:

- explicit with respect to slow waves (for which a great accuracy is expected by engineers, since transportation is the one and only phenomenon of interest),
- implicit with respect to fast waves (for which not so much accuracy is required, since pressure propagation is a usually disregarded phenomenon),
- locally conservative, which makes it ready for adaptive mesh refinement,
- positivity preserving for the density and mass fractions.

The design of the overall implicit-explicit Lagrange-projection method involves many interesting mathematical details. These will be elaborated on in the joint contributing talk by Dr. Q.H. Tran. In this paper, the emphasis will be laid on the motivation and the general philosophy of the proposed technique. Efficiency of the multiresolution method for time adaptive mesh design is also assessed in this setting. Extensive numerical results for realistic test cases are then presented in order to illustrate the capabilities of the resulting method.

Control analysis for water-quality problem. **Mohammed Louaked** (Université de Caen, France) IC/CT1674/025

Analysis of the environmental impact of waste water discharges into aquatic media takes a great importance in the last years. The problem considered here is in the field water-quality improvement by varying the systems, such as flow regulation by means of reservoirs. The creterion functional to be minimized penalizes deviation of phaecal coliforms distribution from standard value. We adress exact and approximate controllability problems for a parabolic equation (evolution of pollutant concentration) associated with Dirac measures.
Hybrid numerical methods combining particle method and finite difference method is presented. Symmetric TVD scheme for the shallow water equations, in general coordinates, is used. The technique is an hybrid method that uses the second order flux in smooth regions but involves some limiting based on the gradient of the solutions so that near discontinuities it reduces to the monotone upwind method. A particle method is proposed to handle the parabolic equation. The difficulty is then to deal with a diffusion term. We analyze an approach based on a purely deterministic method. The approximation of the diffusion operator is based on the introduction of boundary integral equation formulation. The gradient of the cost function is evaluated by adjoint techniques and the quasi-Newton as an iterative solution of the discrete control problem is choosen.
The major issue of the numerical part relies on illustrating by direct simulation the effectiveness of this methodology when applied to the control of water quality problem. Relative merits and advantages of this approach are explored.

Fast algorithms for PDEs in simple and complex geometries. **Prabir Daripa** (Texas A&M University, USA) IC/CT708/026

Solving problems in complex geometries efficiently and accurately are important from practical as well as from fundamental viewpoint. Some numerical methods for solving such problems involve use of domain embedding in combination with fast solvers for regular geometries. The speakers in this minisymposium will describe fast algorithms for regular geometries as well as for complex geometries using a variety of techniques within the above framework. A fast algorithm based on the representation of solutions of PDEs in terms of Green's function in regular geometries and its efficient adaptation for solving problems in complex geometries in combination with domain embedding will also be presented.

Numerical simulation of three-dimensional grain growth in materials containing finely dispersed second-phase particles with the phase field method. **Liesbeth Vanherpe** (Katholieke Universiteit Leuven, Belgium), Nele Moelans (Katholieke Universiteit Leuven, Belgium), Bart Blanpain (Katholieke Universiteit Leuven, Belgium), Stefan Vandewalle (Katholieke Universiteit Leuven, Belgium) IC/CT1889/025

The microstructure of materials often consists of multiple grains with different crystallographic orientations. The study of the evolution of the grains is of great technological importance because many material properties depend on the mean grain size. A common technique to control the grain size of a material is the addition of impurities which leads to the formation of small second-phase particles that will stop the grain growth. The limiting grain size depends on the number, size, shape and spatial distribution of the particles.

We employ a phase field model for simulating three-

dimensional grain growth in materials containing small incoherent second-phase particles which consists of a large set of coupled reaction-diffusion partial differential equations. A fine threedimensional grid is required to resolve the particles and the shape of the grain boundaries. Moreover, a large number of grains and particles should be considered to achieve statistically relevant results. As such, a typical simulation demands extensive computer resources both with respect to memory and computing time.

There are several ways to speed up the computations. We will present two techniques, one using a semi-implicit discretization resulting in an explicit coupling between the partial differential equations so equations can be assigned to different processes and solutions can be computed in parallel. The second technique evolved through a study of the model which revealed that the solutions of the model display small regions of high activity surrounded by large regions of inactivity. This property is exploited through the second technique as we define bounding boxes around the regions of high activity and only solve the equations locally. This algorithm has low memory and computing time requirements.

Multipoint non-local boundary-value problems for Schrödinger equation. **Ali Sırma** (Gebze Institute of Technology, Turkey), Allaberen Ashyralyev (Fatih Üniversitesi, Turkey) IC/CT595/025

In present paper the multi-point nonlocal boundary value problem with integral for Schrödinger equation in a Hilbert space H with the self-adjoint operator A is considered. The stability estimates for the solution of this problem is established. Two multipoint nonlocal boundary value problems with integral are investigated. The first and second order of accuracy difference schemes for the approximate solutions of this nonlocal boundary value problem are presented. The stability of these difference schemes is established. In practice, the stability inequalities for the solutions of difference schemes for Schrödinger equation are obtained. A numerical method is proposed for solving a one-dimensional Schrödinger equation with nonlocal boundary condition. A procedure of modified Gauss elimination method is used for solving these difference schemes. The method is illustrated by numerical examples.

Key Words: Schrödinger equation; Difference schemes; Stability

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IC/CTS4620/02: Numerical methods for PDEs: evolution problems.

Organiser: Miloslav Feistauer (Univerzita Karlova, Czech Republic)
Co-organiser: Richard Sharp (University of Texas at Austin, USA)

Theory and applications of the DGFEM for nonlinear convection–diffusion problems. **Miloslav Feistauer** (Univerzita Karlova, Czech Republic) IC/CT1228/025

In this paper we shall be concerned with several aspects of the numerical solution of convection-diffusion problems by the discontinuous Galerkin finite element method (DGFEM) and applications to compressible flow. The DGFEM is based on a piecewise polynomial approximation of the sought solution without any requirement on the continuity on interfaces between neighbouring elements. It is particularly convenient for the solution of conservation laws with discontinuous solutions or singularly perturbed convection-diffusion problems with dominating convection, when solutions contain very steep gradients.

First subject of our paper is the analysis of L^2-optimal error estimates of the DGFEM applied to nonstationary problems with a nonlinear convection as well as diffusion. The attention will be paid to the DG space semidiscretization and for the DG space discretization combined with backward difference formula used for the time stepping. The theoretical results will be illustrated by numerical experiments.

In the second part, some applications of the DGFEM to the simulation of compressible flow, i.e. the solution of the compressible Euler and Navier-Stokes equations, will be presented. Our goal is to develop sufficiently accurate, efficient and robust numerical schemes allowing the solution of compressible flow for a wide range of Reynolds and Mach numbers. Our approach allows to solve gas flow with practically all Mach numbers (starting from Mach number $= 10^{-6}$ up to transonic regimes). The efficiency and accuracy of the method will be demonstrated by computational results for some technically relevant test problems.

A discontinuous Galerkin approach to the Wigner equation with a non-polynomial basis. **Richard Sharp** (University of Texas at Austin, USA) IC/CT906/024

The dynamics of semiconductor devices and other quantum systems, including interaction with their environment, can be modeled by the Wigner equation and an appropriate collision operator. Previous numerical methods have relied on operator splitting methods. We provide a new approach for simulations built on the Discontinuous Galerkin (DG) method with an arbitrary (non-polynomial) basis. The use of a non-polynomial approximation spaces for DG calculations has recently been proposed by Yuan and Shu. In the context of the Wigner equation, this allows the introduction of a basis tailored to the highly oscillatory solution which develops when a sharp potential is encountered.

Discontinuous Galerkin relaxation algorithm for solute transport in porous media. **Mohammed Mahmood** (Žalinská univerzita, Slovakia) IC/CT3756/025

We consider a degenerate parabolic convection dominated equation which models the transport of contaminant in porous media. The numerical scheme is fulfilled by combining the DG - Discontinuous Galerkin Method with and an efficient relaxation algorithm that recently developed. Numerical results show the efficiency of our scheme.

An accuracy analysis of mass-matrix lumping for 3D unsaturated flow, finite-element, porous-media computations using analytical solutions. **Fred Tracy** (US Army Corps of Engineers, USA) IC/CT433/025

Lumping of the mass matrix for transient problems is the state of the practice for finite element groundwater programs. This improves nonlinear convergence where there is unsaturated flow, but the discovery was made that the accuracy of the results is reduced as much as an order of magnitude for a test problem. This presentation compares results from a recently derived transient three-dimensional (3-D) analytical solution for the given unsaturated flow test problem (Tracy, 2006) with those from a standard parallel Galerkin 3-D finite element groundwater program with the mass matrix lumping option turned both on and off.

A description of the test problem and equations for the analytical solution will also be presented. The test problem consists of transient flow into a rectangular block of initially dry soil until water is applied at the top. Because Richards' equation for describing unsaturated flow in porous media is highly nonlinear, testing is challenging for 3-D finite element groundwater programs. However, accuracy and performance results for these programs can be easily obtained using the analytical solution. Also, the amount of nonlinearity of the analytical solution can be easily adjusted by a parameter α. Accuracy results for various sizes of the mesh and for three values of α of the 3-D test problem from runs made with and without mass matrix lumping are presented. As α is increased, the accuracy of the solution is decreased. Results for grids as large as $161 \times 161 \times 161$ are computed by using as many as 512 processing elements on the U.S. Army Engineer Research and Development Center Major Shared Resource Center Cray XT3.

Finally, this presentation concludes with parallel performance results obtained in the following study.

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Finite-element discretization of parabolic–elliptic interface problems. **Marcus Stiemer** (Universität Dortmund, Germany) IC/CT2783/025

In this presentation mixed boundary value problems for partial differential equations are considered that are parabolic in one part of the underlying domain and elliptic in another part. On the interface of the region of elliptic and parabolic behavior a jump condition for the Neumann traces is given. Such interface problems occur in eddy current simulations in electrodynamics. The fully discrete scheme applied to compute an approximative solution of the mixed problem is based on a spatial discretization with edge elements and a temporally discontinuous Galerkin method. Its convergence is proven and *a priori* error estimates are given. Moreover, adaptive schemes based on *a posteriori* error control are presented.

Efficient numerical schemes for singularly-perturbed parabolic initial boundary-value problems. **Natesan Srinivasan** (IIT Guwahati, India), Rajdeep Deb (IIT Guwahati, India) IC/CT483/025

In this article, we consider the time-dependent singularly-perturbed reaction–diffusion problems of the form $-\varepsilon u_{xx} + b(x,t)u(x,t) + d(x,t)u_t = f(x,t)$, $(x,t) \in (0,1) \times (0,T]$, where $0 < \varepsilon \ll 1$, subject to initial and boundary conditions. These problems arise in several branches of engineering and applied mathematics which include fluid dynamics, quantum mechanics, elasticity, chemical reactor theory, etc. In general, the solution $u(x,t)$ exhibit boundary layers of parabolic type along the sides $x = 0$ and $x = 1$. A careful examination of numerical computations shows that usually the point-wise error in the numerical solution actually increases, as the mesh size $\triangle x$ is refined to the stage where $\triangle x$ is of the same order of magnitude as ε.

To solve these types problems, we propose two efficient numerical schemes. We discretize the domain by using uniform mesh in the time, and piecewise-uniform Shishkin mesh in space. To discretize the spatial derivatives we propose a cubic spline scheme on variable mesh, and apply it on the layer resolving Shishkin mesh. The cubic spline scheme fails to satisfy stability in the outer region. To overcome this difficulty, we use the classical central difference scheme only for the outer region, and the cubic spline scheme for the inner regions. For the discretization of the time derivative we use the Crank-Nickolson scheme and the Extendeded Trapezoidal formula. The newly proposed schemes are of order $O((\triangle t)^3 + (\triangle x)^2)$. The Crank-Nickolson scheme produces nonphysical oscillations near the boundaries when there are inconsistencies in the boundary and the initial conditions. The Extendeded Trapezoidal formula is capable of handling such difficult phenomena. The truncation error, and stability estimates are obtained. The proposed methods are applied to some test problems to verify the theoretical results.

IC/CTS4633/02: Numerical methods for PDEs: evolution problems.

Organiser: Daisuke Furihata (Osaka University, Japan)
Co-organiser: Mauricio Sepúlveda (Universidad de Concepción, Chile)

Simulation of a pollution problem in porous media . **Rajae Aboulaich** (LERMA, Ecole Mohammadia d'Ingénieurs, RABAT, Morocco) IC/CT1916/002

When the ground is accidentally or industrially polluted with a volatile organic pollutant, it is very important to know the amount of this contamination in its liquid form. A relevant question for determining a possible remediation senarii is the ability to characterize the level of the pollution in a short time. We are interested in determination of the concentration in liquid phase of a volatile organic pollutant at initial time, since we can compute its concentration in gaseous phase at final time. This leads to solve an inverse problem (see [1]). We study the existence and uniqueness of solutions for the direct problem in bi-dimensional setting extending the previous work done for uni-dimensional problem [1].

By applying finite volumes method, we discretize the problem and we prove some *a priori* and *a posteriori* error estimates under some suitable conditions. Finally, we globally solve the considered problem by using the finite volumes method.

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Numerical Method for the KdV–Kawahara and Benney–Lin equations. **Mauricio Sepúlveda** (Universidad de Concepción, Chile), Octavio Vera (Universidad del Bío-Bío, Chile) IC/CT4576/025

We are concerned with the initial-boundary-value problem associated to the Korteweg–de Vries–Kawahara (KdVK) and Benney–Lin equations (BL), which are transport equations perturbed by dispersive terms of 5th order. The (KdVK) and (BL) equations appear in several fluid dynamics problems. We obtain local smoothing effects that are uniform with respect to the size of the interval. We also propose a simple finite-difference scheme for the problem and prove its stability. Finally, we give some numerical examples.

Numerical study of coupled surface and grain boundary motion. **Zhenguo Pan** (University of British Columbia, Canada) IC/CT4583/025

We study the coupled surface and grain boundary motion in a bicrystal in the context of the *quarter loop* geometry. Two types of normal curve velocities are involved in this model: motion by mean curvature and motion by surface diffusion. Three curves meet at a single point where junction conditions are given. A formulation that describes the coupled normal motion of the curves and preserves arc length parametrization up to scaling is proposed. Equations and junction conditions are approximated by finite difference methods. Numerical convergence to exact travelling wave solutions is shown.

Application of discrete variational derivative method. **Daisuke Furihata** (Osaka University, Japan) IC/CT2725/025

We have proposed a method to construct numerical schemes for PDEs which have some dissipative or conservative properties.

This method, we refer to it as discrete variational derivative method(DVDM), is a kind of structure preserving methods for PDEs.

The key idea of DVDM is to discretise the variational structure of PDEs which is essence of those properties using rigorous definitions of discrete variational derivative. It follows that constructed schemes inherit the property of integral functional of PDEs.

For example, we are able to construct dissipative or conservative properties preserving schemes for $\partial u/\partial t = (\partial/\partial x)^{\alpha}(\delta G/\delta u)$, $\partial^2 u/\partial t^2 + C\partial u/\partial t = (\partial/\partial x)^{\alpha}(\delta G/\delta u)$ and other kind of PDEs. Examples of concrete PDEs are Swift-Hohenberg equation, Cahn-Hilliard equation, KdV equation, Camassa-Holm equation and so on.

Due to preserving properties we able to expect that those schemes have preferable properties such as numerical stability and solution uniqueness. In fact, we obtained mathematical proofs for such properties of some our schemes.

Not only applying DVDM to PDEs but we also have studied DVDM carefully to extend it, for instance, to obtain higher order of precision, to use other than finite difference method, to apply higher space dimension and so on. We will talk and indicate result of our effort.

IC/CTS4624/02: Numerical methods for PDEs: evolution problems.

Organiser: James Lambers (Stanford University, USA)

Recent advances in Krylov subspace spectral methods. **James Lambers** (Stanford University, USA) IC/CT806/025

This talk summarizes recent and ongoing work on an alternative approach to the solution of diffusion problems and wave propagation problems in the variable-coefficient case that leads to a new numerical method, called a Krylov subspace spectral method.

The basic idea behind the method, applied to a PDE of the form $\mathrm{d}u/\mathrm{d}t + L(x,D)u = 0$, is to use Gaussian quadrature in the spectral domain to compute Fourier components from elements of $\exp[-L\Delta t]$ for a matrix L discretizing $L(x,D)$ and time step Δt, using algorithms developed by Golub and Meurant, as opposed to applying Gaussian quadrature in the spatial domain as in traditional spectral methods. This strategy allows accurate resolution of all desired components, for both high and low frequencies, without having to resort to smoothing techniques to ensure stability. In fact, by viewing the Fourier components in terms of directional derivatives of moments, we can demonstrate unconditional stability given sufficient smoothness of the coefficients of $L(x,D)$.

We also discuss various generalizations of these methods. We first discuss application to systems, which yields a simple high-order scheme for the second-order wave equation. Next, we consider the use of trial functions other than trigonometric polynomials, including smooth, compactly supported wavelets, and multiwavelet bases similar to those introduced by Alpert *et al.*, with differentiation operators designed to compute moments more accurately in the case of discontinuous coefficients. Numerical results will be presented for both parabolic and hyperbolic problems in one, two and three space dimensions.

This talk includes joint work with Patrick Guidotti and Margot Gerritsen.

A central scheme for shallow-water flows along channels with irregular geometry. **Jorge Balbás** (University of Michigan, Ann Arbor, USA), Smadar Karni (University of Michigan, Ann Arbor, USA) IC/CT3025/025

We present a new high-resolution, non-oscillatory semi-discrete central scheme for one-dimensional shallow water flows along channels with non-uniform rectangular cross sections and bottom topography. The scheme extends an existing central semi-discrete formulation for hyperbolic conservation laws and it enjoys two properties crucial for the accurate simulation of shallow water flows: it preserves the positivity of the water height, and it is well balanced, *i.e.*, the source terms arising from the geometry of the channel are discretized so as to balance the non-linear hyperbolic fluxes –a condition necessary to correctly approximate steady-state solutions. Along with a detailed description of the scheme and its properties, we present several numerical experiments –including the approximation of exact equilibrium solutions– that demonstrate the robustness –and simplicity– of the numerical algorithm.

Numerical solution of the time-dependent incompressible Navier–Stokes equations in the stream function and vorticity formulation. **Fattehallah Ghadi** (Université Ibnou Zohr – Agadir, Morocco), Ruas Vitoriano (Université Pierre et Marie Curie, France), Wakrim Mohamed (Département de Math-Info, Faculté des Sciences. Un, Morocco) IC/CT57/025

In this paper we start by presenting the study carried out for the stationary case, and then we link it to the time-dependent case. In terms of numerical analysis this paper primarily deals with a mixed method to solve the two-dimensional generalized Stokes problem. We introduce a suitable technique based on the splitting of the vorticity into two components. Then we discretize in space the resulting uncoupled system by means of continuous Lagrange finite elements. In computational terms we apply the above technique to the Navier-Stokes equations. This is achieved by first performing the semi-discretization in time of these equations by a classical characteristics method or a semi-implicit integration scheme for the advective term. Then we apply the same numerical ingredients as for the generalized Stokes system. Finally we illustrate the good performance of our approach by means of numerical results, obtained in the framework of some benchmarks.

Lagrange projection scheme for two-phase flows: 2. boundary conditions and second-order enhancement. **Quang Huy Tran** (Institut Français du Pétrole, France), Frederic Coquel (Université Pierre et Marie Curie, France), Quang Long Nguyen (Institut Français du Pétrole, France), Marie Postel (Université Pierre et Marie Curie, France) IC/CT2304/025

We are concerned with the numerical simulation of two-phase flows representing oil transportation along a 1-D pipeline. In the joint contributed talk by Q.L. Nguyen, we have discussed about the motivation and the general philosophy of Lagrange-Euler projection method we propose for this kind of problems. In this presentation, we would like to focus on various technical aspects of utmost importance for numerical analysis, namely:

- The design of appropriate boundary conditions for the implicit-explicit Lagrange-projection scheme. Those boundary conditions are based on Dubois-LeFloch's principle of half-Riemann problems.
- An upper-bound for the time-step ensuring positivity properties. This estimate is closely related to a nice structure of the linear system arising in the Lagrange step.
- The construction of a "genuinely" second-order version of the scheme, inside the computational domain as well as on the boundaries. Our approach lies in seeking corrective factors for the slopes from the equivalent equations of the system.

To our knowledge, the proposed methods answer open problems of both practical and theoretical importance. After providing mathematical details for a simplified case of the physical model, relevant numerical results are shown for academic test cases.

Surface-tension driven flows in microfluidics. **Paul Vigneaux** (Université de Bordeaux, France), Cédric Galusinski (Université du Sud-Toulon-Var, France) IC/CT2367/025

Making the most of surface tension effects, flows of two immiscible fluids in microdevices allow to create emulsions where droplets moves through microchannels networks and are used as microreactors to study very fast chemical kinetics. But a better understanding of hydrodynamics inside droplets is needed in order to achieve flow control needed in practical applications. Simulations of such flows raise several numerical difficulties. For instance, surface tension induces time consuming simulations and implies the use of accurate curvature computation, in particular when topological changes occur. An approach to deal with the first point is proposed in the talk "A new stability condition for surface tension-driven flows" of the Minisymposium "Level-Set methods: fluid applications" organized by Y. Tsai.

In this talk, we focus on the second point : bifluid flows with multiple droplets are considered. We use Level Set techniques to follow fluid interfaces. Small droplets are numerically captured with a small number of cells. Then, relative volume variations are visible for such small droplets, even with an efficient level set method. Here we propose to control the volume of each droplet by numerical mass conservation. This obliges namely to locate each droplet, i.e. each connected component represented as connected region where the level set function is, for instance, negative. The number of connected components can vary along time because of topological changes. We then propose an algorithm to isolate each connected component in order to compute and correct the droplet mass. Other applications follow from this algorithm: we can compute the scalar velocity of each droplet in the flow and accurate computation of the curvature can be achieved when two droplets are close. This allows relevant simulations of droplet collapse when surface tension plays a major role. Simulations are compared to physical experiments and different mixing regimes inside microdroplets are explored.

Locally divergence-preserving schemes of higher order. **Robert Artebrant** (ETH Zürich, Switzerland) IC/CT4585/025

Violation of the divergence constraint on the magnetic flux density in magnetohydrodynamical (MHD) simulations leads to stability problems. It is therefore of great importance to numerically respect this intrinsic constraint. Since the divergence preservation is a local phenomenon inherent in the MHD-system it is appealing to mimic this property numerically by a locally divergence-preserving scheme.

A common numerical technique for simulation of the MHD-system of conservation laws is the finite volume (FV) method. In [SISC 26 2005 pp. 1166] a local procedure to redistribute the numerical fluxes in a FV-scheme so that a discrete divergence operator vanishes was presented. This procedure stabilizes the base scheme and respects the accuracy to the second order level.

The present talk describes a development of the above procedure that complies with the finite volume framework, preserves a fourth order discrete divergence operator locally and retains the accuracy of a generic semi-discrete finite volume scheme up to fourth order. The redistribution of the numerical magnetic field fluxes is formulated in a standard conservative setting making it trivial to implement the divergence-preserving modification in an existing FV-scheme.

IC/CTS4594/02: Numerical methods for PDEs: evolution problems.

Organiser: Damian Trif (Universitatea Babeş-Bolyai, Romania)

Characteristic non-reflecting boundary conditions for multi-dimensional quasi-linear hyperbolic systems. **Takaharu Yaguchi** (University of Tokyo, Japan) IC/CT2217/025

We will talk about an extension of the characteristic nonreflecting boundary condition for multidimensional quasi-linear hyperbolic systems, which is important for the simulations of waves.

In these three decades, a variety of nonreflecting boundary conditions have been proposed. Among them, the characteristic nonreflecting boundary condition is widely used for the simplicity of the implementation, but it has a problem that waves are assumed to propagate perpendicular to the boundaries.

In this talk we provide a method to derive characteristic nonreflecting boundary conditions under a weaker assumption that there exist only simple waves. In our method, the coefficients of the equations describing the characteristic curves are adaptively estimated by applying method of characteristics, and

then, reflections are eliminated by a flux vector splitting technique suitable for our method.
We demonstrate the effectiveness of our method by showing numerical examples for the Euler equations and the Maxwell equations.

Local non-reflecting boundary condition for time-dependent multiple scattering. **Imbo Sim** (Universität Basel, Switzerland), Marcus Grote (Universität Basel, Switzerland) IC/CT2478/025

When an incident wave encounters an obstacle, it is scattered in the unbounded surrounding medium. If two or more obstacles are present, the field scattered from one obstacle will induce further scattered fields from all the other obstacles, which again will induce further scattered fields from all obstacles, and so forth. When the scatterer consists of several obstacles, which are well separated from each other, the use of a single artificial boundary to enclose the entire scattering region becomes too expensive. Instead it is preferable to enclose every sub-scatterer by a seperate artificial boundary. Then, any boundary condition for such *multiple scattering problems* must not only let outgoing waves leave a sub-domain without spurious reflection from its artificial boundary, but also propagate subsequently the outgoing wave to all other sub-domains. In [2,3], Grote and Kirsch derived a nonreflecting boundary condition(NBC) for time-dependent multiple scattering, which is local in time but nonlocal in space. Here, based on high-order *local nonreflecting boundary condition*(LNBC) for single scattering [1], we seek a LNBC for time-dependent multiple scattering, which is completely *local both in space and time*. To do so, we first develop a high order representation formula for a purely outgoing wave field, given its values and those of certain auxiliary functions needed for the LNBC on the artificial boundary. By combining that representation formula with the decomposition of the total scattered field into purely outgoing contributions, we obtain the first exact, completely local, NBC for time-dependent multiple scattering. Remarkably, the information transfer (of time retarded values) between sub-domains will only occur across those parts of the artificial boundary, where outgoing rays intersect neighboring sub-domains, i.e. typically only across a fraction of the artificial boundary. The accuracy, stability and efficiency of this new LNBC is evaluated by coupling it to standard finite element and finite difference methods.

key words: time-dependent waves, local nonreflecting boundary condition, local space, local time, multiple scattering

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Email: Marcus.Grote@unibas.ch(Marcus Grote), Imbo.Sim@unibas.ch(Imbo Sim)
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A new high-order finite-volume method for hyperbolic balance laws. **Bettina Messerschmidt** (Universität Kassel, Germany) IC/CT1435/025

Solving PDEs numerically it is often necessary to use methods that guarantee a high order time resolution, especially when the evolution of a process shall be predicted over a longer period.
The already known ADER approach is a way to obtain solutions with a time order greater than one, more precisely it allows convergence of (at least theoretically) arbitrary high order in time. This technique has the disadvantage that for each integration point solving as many Riemann Problems as the designated order is needed, which causes a certain effort in both programming and computing time.
In this talk a new approach will be presented that needs solving only one Riemann Problem per integration point and is much simpler to implement. This procedure is a derivative of the ADER Scheme and uses Taylor Series not only in time but also in space, so that one gets only one value per integration point and side which leads to only one Riemann Problem. A comprehensive comparison of the mentioned numerical schemes in the background of the Shallow Water Equation, with respect to both accuracy and computational effort, will be presented.

Construction of Galerkin schemes that retain energy dissipation or conservation property. **Takayasu Matsuo** (University of Tokyo, Japan) IC/CT1527/025

In this talk numerical integration of a certain partial differential equations (PDEs) that have energy dissipation or conservation property, such as the nonlinear Schrödinger equation, the Korteweg-de Vries equation, or the Cahn-Hilliard equation, is considered. For such PDEs, numerical schemes that retain the energy dissipation or conservation property ("dissipative" or "conservative scheme") are generally prefered in that they often imply physically better and numerically stabler results. Thus so far many studies to seek for dissipative/conservative schemes have been done in this context. Among them, quite recently an unified approach to find dissipative/conservative Galerkin schemes has been proposed by the present author. In this talk, this approach is first briefly reviewed, and its extension and several new application examples of the approach are discussed.

Algorithm and Matlab package for some nonlinear 2D evolution equations. **Damian Trif** (Universitatea Babeş-Bolyai, Romania) IC/CT1251/025

The paper presents an algorithm and the corresponding MATLAB package to solve some partial differential evolution equations of the form $u_t + Lu = N(u, u_x)$, with boundary and initial conditions, where L is a 2D linear elliptic operator and N is a nonlinear part. The algorithm is based on the eigenfunctions expansion together with the Lyapunov-Schmidt reduction procedure. The eigenfunction basis of the linear part L of the problem is used to represent the solution at every time level and these eigenfunctions are calculated in a preprocessing stage. A boundary-fitted computational grid is generated in order to allow a complex geometry of the physical domain and this also facilitates the use of previous 1D versions LiScEig and LiScNLE of the package (D. Trif, LiScEig Tutorial 2005, LiScNLE Tutorial 2006, http://www.mathworks.com/matlabcentral/fileexchange > Mathematics > Differential Equations > LiScEig 1.0 or LiScNLE 1.0). The advantages of such computations can be remarked in many non-trivial examples. Future extensions to free surface problems or blood flow in microcirculation are also discused.

Local and global time-stepping for fully-adaptive multi-resolution methods to solve evolutionary PDEs. **Margarete Domingues** (Instituto Nacional de Pesquisas Espaciais, Brazil) IC/CT750/025

We present a fully adaptive numerical scheme for evolutionary PDEs based on a finite volume discretization. A multiresolution strategy allows local grid refinement while controlling the approximation error in space. The space implementation uses a dynamic tree data structure which allows memory compression and CPU time reduction. The costly fluxes are evaluated on the adaptive grid only. The explicit time discretization, uses either a local scale dependant time step (LTS) or a global time step control (GTS). For the LTS, the time step for the finest scale is imposed by the stability requirement of the explicit second order Runge–Kutta scheme. The time step on a given scale is subsequently twice lager than the one on the next finer scale. For the GTS, a combination of third and second order Runge-Kutta compact schemes are used to control and ajust the time step. Numerical validations are presented for different test problems, like convection-difussion, Burgers equation and Euler equation. To demostrate the efficiency of the different adaptive schemes, we applied them to a non-linear problem in three space dimensions. The gain in memory and CPU time with respect to the finite volume scheme on a regular grid and the adaptive multiresolution method is reported and demonstrates the efficiency and accuracy of such implementations.

IC/CTS4635/02: Numerical methods for PDEs: stationary problems.

Organiser: Jiahn-horng Chen (National Tiawan Ocean University, Taiwan)

Boundary-element method for spatially-periodic potential problems. **Hidenori Ogata** (The University of Electro-Communications, Japan) IC/CT4340/026

In this study, we propose a boundary element method (BEM) for two-dimensional potential problems with one-dimensional periodicity such as electrostatic problems including an infinite periodic array of electric conductors. The conventional BEM is based on boundary integral equations. It is, however, difficult to solve periodic problems by the conventional BEM because the solution, which includes periodic functions, is difficult to be obtained by solving the integral equation including the Green function due to an isolated source. We propose a BEM based on a "periodic" Green function, a Green function due to a periodic array of sources, which successfully provides approximate solutions of periodic potential problems.

A reduction approach of mixed finite element methods in magnetic fields problems. **Daisuke Tagami** (Kyushu University, Japan) IC/CT3219/026

We are concerned here with finite element computations of magnetic field problems; for example, three-dimensional eddy current problems using the magnetic vector potential as an unknown function. By introducing a mixed formulation with the gauge condition, we can mathematically justify the existence and unique solvability, and the convergence of the approximate solution; for example, see[3] in the magnetostatic case. However, the mixed formulations cause the difficulty to apply iterative solvers to the resultant linear systems. This fact makes one of the main disadvantage in the practical computations for large scale models of electric facilities. On the other hand, a formulation without the gauge condition (hereafter, we call “reduction approach”) is often used, where it is known that the convergence of iterative solvers is improved by taking care of the continuity of an excitation current density; for example, see[1] and[2]. However, in “reduction approach”, the unique solvability is disregarded.

Therefore, in this paper, we focus our attention on mathematical justifications of “reduction approach”, which means to prove the existence and unique solvability, to prove the convergence, and to find the relation between the constraint condition of the mixed problem and “reduction approach”.

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Applications of RBF collocation method to elliptic PDEs in an arbitrary domain by fictitious domain extensions. **Jiahn-horng Chen** (National Tiawan Ocean University, Taiwan) IC/CT371/026

It is known that the multiquadric functions possess the best capability in scattered data fitting and their convergence is of exponential order. Recently, the multiquadric radial basis function (RBF) collocation method has been widely applied to solve partial differential equations. The applications are usually restricted to simple domains. However, the geometries of problems in industry and engineering are almost always irregular and complicated. To employ the RBF collocation method to solve a problem in an arbitrary domain, one usually needs to incorporate some domain decomposition techniques in a typical solution procedure. In this way, iterations are required.

In this paper, we introduce a fictitious domain extension approach that extends the arbitrary physical geometries defined in a problem to a topologically rectangular domain. In this approach, the definitions of the solution function and its governing equation are extended to the fictitious region and its boundary. The physical boundary conditions are still specified on the boundaries of the physical domain. And then the RBF collocation method is applied in the new extended domain. Applying this approach to several test problems with arbitrary geometries, we demonstrate that the solution can be directly obtained without domain decompositions and iterations. We also tested the approach for problems with different types of boundary conditions. The results show that the new approach is simple, efficient and accurate.

The composite mini-element: a mixed FEM for the Stokes' equations on complicated domains. **Daniel Peterseim** (Universität Zürich, Switzerland), Stefan Sauter (Universität Zürich, Switzerland) IC/CT3293/026

In this talk, we introduce a new mixed finite element for the discretization of the Stokes equations with Dirichlet as well as slip boundary conditions. The underlying grids of the standard finite element pairs, like the well-known Mini Element, always has to resolve the domain which affects the number of degrees of freedom critically. In contrast to that, our approach decouples the minimal dimension of the approximation space from the domain geometry by using an overlapping two-scale grid. This approach allows low-dimensional approximations even for problems with complicated geometric details. We prove stability and optimal convergence for the proposed nonconforming mixed method.

A complete flux scheme for the stationary advection-diffusion-reaction equation. **Jan ten Thije Boonkkamp** (Technische Universiteit Eindhoven, The Netherlands) IC/CT2415/026

We derive the complete flux scheme for conservation equations of advection-diffusion-reaction type, which can be considered as a generalization of exponential fitting schemes. The advection velocity, diffusion coefficient and source term can be arbitrary smooth functions. In the complete flux scheme, the numerical flux at a cell interface is computed from the complete differential equation, including the source term. This way we get a numerical flux consisting of two parts, i.e., the homogeneous flux, corresponding to the advection-diffusion operator, and the inhomogeneous flux, corresponding to the source term. For two-dimensional problems we include the cross flux in the source term. The numerical flux behaves second order accurate, uniformly in the local Peclet numbers. We have combined the complete flux scheme with the cell-centred finite volume method, and the resulting scheme is second order accurate and not prone to spurious oscillations, even for dominant advection. Moreover, for two-dimensional problems crosswind diffusion is virtually absent. Finally, we have modified the scheme for the spherically symmetric advection-diffusion-reaction equation.

An augmented discontinuous Galerkin method for elliptic problems. **Rommel Bustinza** (Universidad de Concepción, Chile), Tomas Barrios (Universidad Católica de la Santisima Concepción, Chile) IC/CT3097/026

In this work we propose an augmented discontinuous Galerkin method for elliptic linear problems in the plane with mixed boundary conditions. Our approach introduce Galerkin least-squares terms, arising from constitutive and equilibrium equations, which allow us to look for the flux unknown in the local Raviart-Thomas space. The unique solvability is established avoiding the introduction of lifting operators and we derive a Céa estimate, which let us conclude that the rate of convergence of error, measured in an appropriate norm, is optimal respect to the $h-$version. We emphasize that for practical computations, this method reduces the degrees of freedom, with respect to the classical discontinuous Galerkin method. In addition, an aposteriori error analysis is presented and some numerical experiments are included, which validate our theoretical results.

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IC/CTS4623/02: Numerical methods for quadrature.

Organiser: Jörg Waldvogel (ETH Zürich, Switzerland)

Variable transformations in numerical integration. **Avram Sidi** (Technion – Israel Institute of Technology) IC/CT3991/022

Consider the problem of evaluating finite-range integrals of the form

$$I[f] = \int_0^1 f(x)\,dx,$$

where $f \in C^\infty(0,1)$, but $f(x)$ may behave singularly at the endpoints with different types of singularities. One very effective way of computing $I[f]$ is by first transforming it with a suitable variable transformation and next applying the trapezoidal rule to the resulting transformed integral. Thus, if we make the substitution $x = \psi(t)$, where $\psi(t)$ is an increasing differentiable function on $[0,1]$, such that $\psi(0) = 0$ and $\psi(1) = 1$, then the transformed integral is

$$I[\hat{f}] = \int_0^1 \hat{f}(t)\,dt; \quad \hat{f}(t) = f(\psi(t))\psi'(t).$$

If $\psi(t)$ is chosen such that $\psi^{(i)}(0) = \psi^{(i)}(1) = 0$, $i = 1,2,\ldots,p$, for some sufficiently large p, then the trapezoidal rule applied to $I[\hat{f}]$ produces approximations of surprisingly high accuracy even with a small number of abscissas.

Variable transformations in numerical integration have been used as a means to improve the performance of the trapezoidal rule and of the Gauss–Legendre quadrature for singular one-dimensional integrals. They have also been used in multidimensional integration to "periodize" the integrand in all variables to improve the accuracy of lattice rules.

In this lecture, we give an overview of the subject. We discuss the various transformations, old and new. We present some recent developments that enable one to obtain "optimal" numerical results from some transformations that have power-like behavior at the endpoints.

Fast construction of the Fejér and Clenshaw–Curtis quadrature rules. **Jörg Waldvogel** (ETH Zürich, Switzerland) IC/CT4087/022

We present an elegant algorithm [1] for stably and quickly generating the weights of Fejér's quadrature rules and of the Clenshaw–Curtis rule. The weights for an arbitrary number of nodes are obtained as the discrete Fourier transform of an explicitly defined vector of rational or algebraic numbers. Since these rules have the capability of forming nested families, some of them have gained renewed interest in connection with quadrature over multi-dimensional regions.

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About some quadrature formulae. **Zlatko Udovičić** (University of Sarajevo, Bosnia and Herzegovina) IC/CT944/022

In paper[1] the authors considered the quadrature formulae of the form:

$$\int_0^{N-1} \phi(x) f(x) \mathrm{d}x \approx \sum_{i=1}^{r} w_i f(d_i - \tau),$$

where $\phi(\cdot)$ is a scaling function supported on the interval $[0, N-1]$, d_i are the points from the diadic scale, while the unknown parameters of this formula are weights w_i and shift τ. To obtain better numercial stability, instead of the standard polynomial base, the authors used Chebyshev polynomials of the first kind. We generalized that idea and developed algorithms for using any other orthogonal polynomials. Some numerical examples are also presented.

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Quadrature formulae with maximal trigonometric degree of exactness. **Marija Stanić** (Univerzitet u Kragujevcu, Yugoslavia), Gradimir Milovanović (Univerzitet u Nišu, Yugoslavia), Aleksandar Cvetković (Univerzitet u Nišu, Yugoslavia) IC/CT4355/022

In this lecture we consider quadrature formulae of interpolatory-type, with multiple nodes, which have maximal trigonometric degree of exactness. Our approach is based on procedure given by Ghizzeti and Ossicini in [Quadrature Formulae, Academie-Verlag, Berlin, 1970.]. We consider $\sigma-$orthogonal trigonometric polynomials of semi-integer degree, and give numerical method for their construction. Also, some numerical examples are included.

Quadratures with respect to the complex Jacobi weight. **Gradimir Milovanović** (Univerzitet u Nišu, Yugoslavia), Aleksandar Cvetković (Univerzitet u Nišu, Yugoslavia) IC/CT4371/002

We consider quadrature formulae of the form

$$\int_{-1}^{1} f(x)\, w(x)\, \mathrm{d}x = \sum_{k=1}^{n} A_k f(x_k) + R_n(f),$$

where $w(x) = (1-x)^{\alpha}(1+x)^{\beta}$ is the Jacobi weight function with complex parameters α and β, such that their real parts greater than -1. Such type of integrals appear in some problems of theoretical physics (*cf.* I. Mancev, Journal of Computational Methods in Sciences and Engineering **5** (2005), pp.73–89).

We derive Gaussian type of quadratures, as well as some other kind of interpolatory formulas. We discuss questions of construction and convergence for such formulas and give some numerical examples.

Gaussian quadratures using values-of-function derivatives. **Aleksandar Cvetković** (Univerzitet u Nišu, Yugoslavia), Gradimir Milovanović (Univerzitet u Nišu, Yugoslavia) IC/CT4373/022

In this talk we consider quadrature rules of the following type

$$\int p d\mu = \sum_{k=1}^{n} w_k((q(D)D^m)p)(x_k),$$

where q is given polynomial with $q(0) = 1$ and D is the derivative operator. We discuss existence of such quadrature rules exact on the polynomial space $\mathcal{P}^{\lambda}_{2n+m-1}$, where

$$\mathcal{P}_{2n+m-1} = \{p \in \mathcal{P}_{2n+m-1} \mid (D^k p)(\lambda) = 0,\ k = 1, \ldots . m-1\}.$$

Quadrature rules of such type with maximal algebraic degree of exactness are called Gaussian quadrature rules using values of function derivatives.

IC/CTS4628/02: Numerical methods for PDEs: stationary problems.

Organiser: Christos Xenophontos (University of Cyprus)
Co-organiser: Marcus Sarkis (WPI/USA and IMPA/Brazil)

Why finite element discretizations can be factored by triangular hierarchical matrices. **Mario Bebendorf** (Universität Leipzig, Germany) IC/CT4381/026

Although the asymptotic complexity of direct methods for the solution of large sparse finite element systems arising from second-order elliptic partial differential operators is far from being optimal, these methods are often preferred over modern iterative methods. This is mainly due to their robustness. In this talk it is shown that an (approximate) LU decomposition can be computed in the algebra of hierarchical matrices with logarithmic-linear complexity and with the same robustness as the classical LU decomposition.

An important application of low-precision approximants are preconditioners. It will be seen from both, analysis and numerical experiments, that a problem independent number of iterations can be guaranteed.

The approximation by hierarchical matrices relies on a so-called admissibility condition which is a geometric condition on the localisation of the degrees of freedoms associated with the rows and columns of each subblock. Since this condition is only sufficient, we will generalize it to a purely algebraic condition and prove existence of approximants.

BDDC preconditioners for DG discretizations of elliptic problems with discontinuous coefficients. **Marcus Sarkis** (WPI/USA and IMPA/Brazil), Maksymilian Dryja (Warsaw University, Poland), Juan Galvis (IMPA, Brazil) IC/CT2789/026

Discontinuous Galerkin (DG) discretizations are becoming more and more popular for approximating PDEs since they are well suited for dealing with local or patch refinements and regions with complex geometries or with discontinuous coefficients. We consider DG discretizations for a second order elliptic equation with discontinuous coefficients. The domain Ω is defined as a geometrical conforming union of polygonal substructures Ω_i of size $O(H_i)$. Inside each substructure Ω_i, a triangulation $T_{h_i}(\Omega_i)$ with a h_i parameter and a conforming finite element method are introduced. To handle the nonmatching meshes across $\partial\Omega_i$, we consider DG discretizations based on symmetrized interior penalty terms on the $\partial\Omega_i$. In the first part of the talk a summary on apriori error estimates is presented for the case where the coefficients are constant inside the substructures Ω_i and possibly highly discontinuous across $\partial\Omega_i$. In the second part of the talk, we discuss BDDC solvers based on special orthogonal decompositions of the unknown variables. Under natural assumptions among the coefficients and mesh sizes across $\partial\Omega_i$, a condition number estimate $C(1 + \max_i \log^2 \frac{H_i}{h_i})$ for the preconditioned system is established with C independent of h_i, H_i and the jumps of the coefficients. The algorithms are well suited for parallel computation and can be straightforwardly extended to 3-D problems. Numerical experiments are presented.

An alternating direction Galerkin method for some nonlinear problems. **Sum Chow** (Brigham Young University, USA) IC/CT4377/026

Several problems in porous medium flows and glaciology involve the solution of partial differential equations with gradient dependent nonlinearity. The numerical solution of the resulting nonlinear system is rather expensive. In this paper, we present an alternating direction Galerkin method that allows much faster solution of the nonlinear system.

Our approach is fairly general in scope and covers many problems appearing in diverse application areas. The alternating direction formulation help reduce the problem into a sequence of nonlinear systems that may be solved very efficiently. One special feature of the method is that in for the nonlinear system related to each direction, the solution method is closer to a direct solve than an iterative approach. Theoretical study of the convergence of the method will also be presented.

A singular function boundary integral method for elliptic problems with boundary singularities. **Christos Xenophontos** (University of Cyprus) IC/CT1110/002

We consider a singular function boundary integral method for the approximation of two-dimensional Laplacian problems with boundary singularities due either to the geometry of the domain or to changes in the boundary conditions. In this method, the approximation is constructed by truncating the asymptotic expansion for the solution near the singular point and the Dirichlet boundary conditions are weakly enforced by means of Lagrange multiplier functions. The resulting discrete problem is posed and solved on the boundary of the domain, away from the point of singularity, hence the dimension of the problem is reduced by one. In this talk we will present the numerical analysis of the method, and in particular show that the method approximates the generalized stress intensity factors, i.e., the coefficients in the asymptotic expansion, at an exponential rate. Numerical examples illustrating the convergence of the method and its extension to other elliptic problems with singularities will also be presented.

Non-polynomial spline methods for solving a fourth-order parabolic equation. **Arshad Khan** (Jamia Millia Islamia, New Delhi, India) IC/CT4701/026

In this paper a fourth-order parabolic partial differential equation, that governs the behaviour of a vibrating beam, is solved by using a three level method based on non-polynomial quintic spline in space and finite difference discretization in time. Stability analysis of the method has been presented. It is shown that by choosing the parameters suitably most of the methods can be derived from our method. We also obtain two new high accuracy schemes of $O(k^4, h^6)$ and $O(k^4, h^8)$ and two new schemes which are analogues of Jain's formula for the non-homogeneous case. Comparison of our results with some known methods show the superiority of the present approach.

On the projection to a certain convex set in $H_0^1(\Omega)$, II. **Tomoyuki Idogawa** (Shibaura Institute of Technology, Japan) IC/CT2980/061

Let Ω be a bounded domain with a smooth boundary and $K := \{v \in H_0^1(\Omega) \mid \|\nabla v\|_{L^\infty(\Omega)} \leq 1\}$. In a variational treatment of elasto-plastic torsion problem, the projection mapping $P_K : H_0^1(\Omega) \to K$ plays an important role. We had already showed an iteration algorithm to get $P_K u$ for 1-dimensional case $\Omega = (a, b)$, in the ICIAM-99. We will consider higher dimensional cases and will talk about some related topics.

IC/CTS4640/02: Mesh generation, adaptive methods, multigrid.

Organiser: Wael Elleithy (Universität Linz, Austria)
Co-organiser: Andrei Drăgănescu (Univ. Maryland at Baltimore County, USA)

An abstract method for extending two-level preconditioners to multilevel preconditioners of comparable quality. **Andrei Drăgănescu** (Univ. Maryland at Baltimore County, USA) IC/CT2564/027

We present an abstract method for designing a multilevel preconditioner given a two-level preconditioner for an operator with positive definite symmetric part.

If we denote by A_{fine} and A_{coarse} two discrete versions of a continuous operator, then a two-level preconditioner T_{fine} for A_{fine} is generally described by

$$T_{\text{fine}} = \mathcal{F}(A_{\text{coarse}}^{-1}, A_{\text{fine}}) \approx A_{\text{fine}}^{-1}\,, \qquad (1)$$

where it is assumed that the evaluation of $\mathcal{F}$ requires a level-independent number of applications of A_{fine} and k applications of A_{coarse}^{-1} ($k = 1$ or 2). The natural extension to a multilevel preconditioner, consisting in replacing the call to A_{coarse}^{-1} in (1) with a recursive call to $\mathcal{F}$, is known to sometimes produce multilevel preconditioners of lower quality (e.g., for certain types of inverse problems). Based on the idea that inverting A_{fine} essentially means to solve the nonlinear equation $X^{-1} - A_{\text{fine}} = 0$, we define our multigrid preconditioner to be the first Newton iterate of the map $X \mapsto X^{-1} - A_{\text{fine}}$ starting at the "natural" multilevel preconditioner. For $k = 1$, the resulting algorithm has a W-cycle structure, and differs only slightly from the textbook version of the W-cycle. Moreover, the method guarantees that the resulting preconditioner maintains the approximation quality of the initial two-level preconditioner. The quality of approximation is measured using a distance function that measures the degree to which two operators with positive definite symmetric parts are spectrally equivalent. We apply this method to designing and analyzing a multigrid preconditioner for a linear advection-diffusion-reaction equation.

On a stable coupling approach to multiscale simulations. **Konstantin Fackeldey** (Universität Bonn, Germany), Rolf Krause (Universität Bonn, Germany) IC/CT2720/008

We present a stabilized coupling approach for the multiscale simulation of nonlinear processes in mechanics using finite elements and molecular dynamics concurrently. The key idea is to construct a transfer operator between the different scales on the basis of weighted local averaging instead of using point wise taken values. The local weight functions are constructed by assigning a partition of unity to the molecular degrees of freedom. This allows for decomposing the micro scale displacements into a low frequency and a high frequency part by means of a weighted $L2$-projection. As a consequence, spurious modes are eliminated by construction of the transfer operator. Numerical experiments illustrating the stabilizing effect of our coupling approach are given.

Two-level preconditioners for 3D flows in highly-heterogeneous porous media. **Iryna Rybak** (Fraunhofer ITWM, Kaiserslautern, Germany), Richard Ewing (Texas A&M University, USA), Oleg Iliev (Fraunhofer ITWM, Kaiserslautern, Germany), Raytcho Lazarov (Texas A&M University, USA) IC/CT4432/027

The talk concerns two-level DD/MG type preconditioners for 3D pressure equation with highly varying discontinuous scalar and tensor coefficients. Multipoint flux approximation approach is used for finite volume discretization of the boundary value problem. The domain is divided into nonoverlapping subdomains (blocks), and two-level domain decomposition preconditioners are considered. The heterogeneities are not resolved by the coarse blocks boundaries, therefore the choice of the coarse grid operator is a non-trivial task. The choice of the interlevel operators is also critical for the convergence of the method. The coarse scale operator used here is derived via the homogenization approach. Solutions of local auxiliary problems (so called cell problems) are postprocessed in order to upscale the permeability tensor. Different types of boundary conditions for the cell problems are studied. Namely, these are periodic, linear, oscillatory and Neumann boundary conditions. In the case of periodic porous media, all these boundary conditions allow to calculate one and the same upscaled permeability tensor. However, if the medium is not periodic, different boundary conditions for the auxiliary cell problems lead to different block permeability tensors, what in turn may influence the convergence of the two level DD iterative method. This influence is numerically studied on various types of non-periodic porous media. The influence of the oversampling is studied as well. Furthermore, different choices for a smoothing procedure are studied. These are overlapping and non-overlapping Schwarz DD methods as well as ILU. Results from numerical experiments are presented in order to demonstrate the performance of the considered two-level DD preconditioners.

FEM–BEM coupling for elasto-plastic analysis: automatic adaptive generation of the FEM and BEM zones of discretization. **Wael Elleithy** (Universität Linz, Austria), Ulrich Langer (Universität Linz, Austria) IC/CT3404/027

The intention of coupling the finite element method (FEM) and the boundary element method (BEM) is to combine the advantageous properties of both discretization methods.

The theory and algorithms of coupling FEM and BEM solutions reached, by now, a fairly matured state. However, existing FEM-BEM coupling approaches requires *a priori* defined zones of discretization (FEM and BEM sub-domains). Furthermore, the predefined FEM and BEM zones of diecretization do not change during the computation. As a consequence, the plastic zone (finite element zone of discretization) must be manually localized in advance. This requires preliminary expert knowledge about the problem at hand and may limit the general applicability of the coupling method. The computational cost can be higher than necessary depending on the definition of the finite element and boundary element zones of discretization (FEM and BEM sub-domains).

In this work, we present the concept and the implementation issues for an adaptive FEM-BEM coupling method for two-dimensional elasto-plastic analysis. The nonlinearity, e.g., plastic material behavior, is treated by the finite element method while large parts of the finite/infinite linear elastic body are treated using the boundary element method. The FEM sub-domain discretization is progressively adapted and automatically generated to include zones where plasticity occurs, according to the state of computation. The substantial decrease in the size of FEM meshes, plainly leads to reduction of required system resources and gain in efficiency. Moreover, higher accuracy is achieved.

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02: Numerical Analysis, Posters

IC/PP388/002: **Optimal long-distance transport systems in nature: control and applications.**

Presenter: Natalya Kizilova (Kharkov Polytechnic University, Ukraine)

Long-distance conducting systems in high plants and animals are presented by networks of either rigid tubes with porous walls (in plants) or distensible tubes with impermeable walls (in animals). Geometrical relations between the diameters, lengths and branching angles of separate conducting vessels have been studied on morphometric data for the intraorgan arterial systems of a human and by computer-assisted image analysis of plant leaf venation [1]. Some results of the comparative analysis are presented. It was shown that the relationships between the geometrical parameters of the transport systems are similar in animals and plants and correspond to the optimal pipelines with impermeable and permeable walls accordingly. The optimization criterion is the total energy expenses W for the liquid delivery and construction of the system. Global optimality at the systemic level is provided by local optimality conditions in each conducting element. The self-similar branching systems with/without anastomoses are considered here as the models of the transport systems in different inner organs of animals and different venation type of the plant leaves. Steady and unsteady flows of a viscous liquid in the systems with permeable/impermeable walls are investigated [2]. Some important features of the conducting systems which are optimal in the meaning of the criterion $W \rightarrow min$ are revealed. It is shown that complexity of the branching system of the optimal tubes leads to certain regularities in the hydraulic and wave properties of the systems. Hydraulic conductivity of the systems with anastomoses is less than the conductivity of the tree-like systems even at the constant total volume of the material that is used for construction of the system. Both hydraulic conductivity and wave admittance of the system decrease when they are considered as functions of the longitudinal coordinate along the branching system. Reflection coefficient G (ratio of the amplitudes of the forward and backward waves) is an increasing function of the longitudinal coordinate in the way that G<0 for the tubes with initial branching orders (n=1-4). That implies that construction and complexity of the biological long-distance transport systems provide relatively low conductivity for the steady liquid flow and negative reflections and active sucking of the liquid for the wave flow through the system. Possible biomedical and technical applications of the revealed regularities are discussed.

[1] Kizilova N.N. (2004) Computational approach to optimal transport network construction in biomechanics. Lecture Notes in Computer Science. vol.3044. pp.476-485. [2] Kizilova N.N. (2005) Hydraulic Properties of Branching Pipelines with Permeable Walls. International Journal of Fluid Mechanics Research. vol.32,N1. pp.98-109.

IC/PP4295/020: **Numerical stability of inexact saddle-point solvers.**

Presenter: Pavel Jiránek (Czech Academy of Sciences, Czech Republic)
Co-author: Miro Rozložník (Czech Academy of Sciences, Czech Republic)

Non-symmetric saddle-point problems arise in a wide variety of applications in computational science and engineering. The aim of this presentation is to discuss numerical behavior of several nonsymmetric iterative methods applied for solving the saddle point systems via the Schur complement reduction or the null-space projection approach. Krylov subspace methods often produce the iterates which fluctuate rather strongly. Here we address the question whether large intermediate approximate solutions reduce the final accuracy of these two-level (inner-outer) iteration algorithms. We distinguish between three mathematically equivalent back-substitution schemes which lead to a different numerical behavior when applied in finite precision arithmetic. Theoretical results are then illustrated via numerical examples.

IC/PP547/020: Solution of dense linear systems with wavelet preconditioned GMRES.

Presenter: Lilian Villarín Pildaín (Universidad de La Habana, Cuba)

The solution of dense linear systems of Great Dimensions is generally achieved by direct methods as the tringular factorizations. Pro's: They are *exact* in infinite arithmetic. Con's: In a finite arithmetic, they may be unstable and, when N is too big, really expensive. That's why we try to apply iterative (Krilov) methods for solving them, preconditioning whith an incomplete factorization. To obtain the preconditioner P cheaply, we need a sparsity pattern that approximates the original dense matrix, and that's why we use compression by wavelet bases.

IC/PP4306/021: Deficient discrete C^1 quartic spline interpolation.

Presenter: Pushpraj Choudhary (Govt. Science College, Jabalpur, India)

A discrete spline of certain degree is a piecewise polynomial function of same degree with smoothness at mesh point being expressed in terms of differences rather than continuity of the derivative by Lyche (BIT, 16 (1976), 281-290). Discrete spline has been introduce by Mangasarian and Schumaker (SIAM. J. Conntrol, 9(1971), 174-183) in connection with the solution of certain minimization problem involving differences. Existence uniqueness and convergence properties of discrete cubic spine interpolating a given function at one intermediate point between the successive mesh points are studied by Rana (Proc. of the Japan Acad., 66(1990), 84-88), Dikshit and Rana (Rocky Mountain J. of Math, 17(1987), 709-718) which extend the result of Dikshit and Power (Numer, MAth., 40(1882), 71-78) for discrete cubic spline interpolation. Rana and Dubey (J. Approx.-Theory, 86(1996), 120-127) have obtained assymptotically precise of the difference between the discrete cubic spline interpolation and the function interpolate, which is some times used to smooth histrogram. It has been observed that the deficient spline are more applicable than usable spline as they require less continuity requirement at the mesh points.

In the present paper, we have studied the existence uniqueness and error estimate of deficient discrete C^1-quartic spline interpolation which match the given function values at three intermediate points between the successive mesh point along with two appropriate boundary conditions which are the preferable some to achieve higher accuracy than lower degree splines in which more data are required.

IC/PP4718/021: Multi-frame image super-resolution using self-examples.

Presenter: Mehran Ebrahimi (University of Waterloo, Canada)
Co-author: Edward Vrscay (University of Waterloo, Canada)

We propose a novel multi-frame super-resolution algorithm using our so called *self-examples'*.

The problem of recovering a high-resolution image from a set of distorted (e.g., warped, blurred, noisy) and lower resolution images is known as super-resolution. It is well known that super-resolution is an ill-posed inverse problem, and the effort of the researchers in the past two decades has been mostly focused on defining more efficient regularization expressions to address this ill-posed inverse problem. Furthermore, accuracy of the existing motion estimation algorithms, commonly required in super-resolution algorithms, is always a bounding limit. In 2005, Buades et. al, proposed a novel denoising technique (known as NL-means) for image sequences which does not require motion estimation by taking advantage of the fact that many pixels in the neighboring frames are similar to the current pixel one wishes to denoise. Furthermore, a new class of example-based super-resolution techniques has been very promising in the past few years. However, an external database of examples is typically required for these example-based techniques prior to reconstruction step.

In our super-resolution method, similar to the NL-means multi-frame denoising, no motion-estimation is required. We perform regularization by taking patches from the image sequence itself. However, as opposed to the NL-means multi-frame denoising, patches are taken at different scales, and not at the same scale, allowing us to perform super-resolution.

IC/PP3046/023: An explicit/implicit Galerkin domain-decomposition procedures for parabolic integro-differential equations.

Presenter: Debasish Pradhan (IIT Bombay, India)
Co-author: Neela Nataraj (IIT Bombay, India)
Co-author: Amiya Pani (IIT Bombay, India)

Variational methods are presented for solving approximately a parabolic integro-differential equation that has elliptic part of order $2m$. In this paper, a non-iterative domain decomposition procedure for parabolic integro-differential equation is discussed. The purpose of this paper is to provide the numerical methods for solving the parabolic integro-differential equations by non-overlapping domain decomposition type techniques, introduced by Dawson.

Based on an implicit Galerkin procedures we are solving inside the sub-domains and explicitly calculate the flux value at the interface (i.e., inter-domain boundaries). *A priori error* estimates are derived and the result of a numerical experiment is presented.

IC/PP780/024: Fast and accurate integration of enzyme kinetics equations.

Presenter: Bruno Bieth (Purdue University, USA)
Co-author: Raymond Chin (Indiana University & Purdue University, USA)
Co-author: Lang Li (Indiana University, USA)

Enzyme kinetics equations have positive solutions with multi-scale structure. To solve these equations accurately and efficiently, we developed two fast integration methods in contrast to existing stiff-ODE solvers. Both methods employ an equivalent system of nonlinear Volterra integral equations so derived by using quasi-linearization and by incorporating initial conditions into the equations. This formulation ensures that the solution is always positive. The difference between these two methods lies in the solution procedure. In one, we use orthogonal polynomial associated to an exponential weight, $e^{-\beta t}$ and while in the other we use successive approximation. In this poster session, we report computations using MAPLE of these methods for the enzyme kinetic equations and their errors compared to standard stiff solvers.

IC/PP2596/024: Software library of Taylor series for differential equation.

Presenter: Hiroshi Hirayama (Kanagawa Institute of Technology, Japan)

The arithmetic operations and functions of the Taylor series can be defined by Fortran, C++ and C# language easily. The functions represented by this language can be expanded in the Taylor series. The solution of the differential equations (DE) can also be expanded in the Taylor series.

The software library of Taylor series is developed for the differential equation (DE). The inverse function of $f(x)$ is satisfy the following equation.

$$\frac{dy}{dx} = \frac{1}{\frac{df(y)}{dy}}$$

Using above, the inverse function can easily be expanded in the Taylor series. Therefore we can expand many kinds of function in the Taylor series.

For examples, the solution of the following differential eqaution

$$\frac{dy}{dx} = -\frac{1}{3}x^2y^2, \quad y(2) = 1$$

can be developed in the Taylor series. The first 10 terms of this Taylor series is as follows.

$$\begin{aligned} y(x) \quad &= 1 - 1.33333 * (x-2) + 1.11111 * (x-2)^2 - 0.703704 * (x-2)^3 \\ &+0.345679 * (x-2)^4 - 0.115226 * (x-2)^5 + 0.00137174 * (x-2)^6 \\ &+0.0365798 * (x-2)^7 - 0.0368846 * (x-2)^8 + 0.0246406 * (x-2)^9 \end{aligned}$$

IC/PP1049/024: A high-order energy-conserving integrator.

Presenter: Yuji Ishimori (Toyama Prefectural University, Japan)

We present a numerical integration scheme for the equations of motion

$$\frac{dp_i}{dt} = -\frac{\partial H}{\partial q_i}, \quad \frac{dq_i}{dt} = \frac{\partial H}{\partial p_i} \quad (i = 1, \cdots, d)$$

with the Hamiltonian $H = H(p_1, \cdots, p_d, q_1, \cdots, q_d)$. The enerygy-conserving scheme of order $2n$ is given by

$$p_i^{k+1} = p_i^k - \sum_{j=1}^{n} c_j \sum_{m=1}^{s_j} I_{Q_{ij}}^{\frac{m}{s_j}, \frac{m-1}{s_j}}, \quad q_i^{k+1} = q_i^k + \sum_{j=1}^{n} c_j \sum_{m=1}^{s_j} I_{P_{ij}}^{\frac{m}{s_j}, \frac{m-1}{s_j}}$$

$$P_{ij}^{k+\frac{m}{s_j}} = \frac{s_j - m}{s_j}(p_i^k - \sum_{l=1}^{m} I_{Q_{ij}}^{\frac{l}{s_j}, \frac{l-1}{s_j}}) + \frac{m}{s_j}(p_i^{k+1} + \sum_{l=m+1}^{s_j} I_{Q_{ij}}^{\frac{l}{s_j}, \frac{l-1}{s_j}})$$

$$Q_{ij}^{k+\frac{m}{s_j}} = \frac{s_j - m}{s_j}(q_i^k + \sum_{l=1}^{m} I_{P_{ij}}^{\frac{l}{s_j}, \frac{l-1}{s_j}}) + \frac{m}{s_j}(q_i^{k+1} - \sum_{l=m+1}^{s_j} I_{P_{ij}}^{\frac{l}{s_j}, \frac{l-1}{s_j}})$$

$$P_{ij}^k = p_i^k, \quad Q_{ij}^k = q_i^k, \quad P_{ij}^{k+1} = p_i^{k+1}, \quad Q_{ij}^{k+1} = q_i^{k+1}$$

$$(k = 0, 1, 2, \cdots; i = 1, \cdots, d; j = 1, \cdots, n; m = 1, \cdots, s_j - 1)$$

where $s_1, \cdots, s_n$ are arbitrary positive integers satisfying the condition

$$s_1 < s_2 < \cdots < s_n,$$

$c_1, \cdots, c_n$ are the weights given by

$$c_j = \frac{s_j^{2n-2}}{\prod_{\substack{l=1 \\ (l \neq j)}}^{n} (s_j^2 - s_l^2)} \quad (j = 1, \cdots, n; n \geq 2)$$

and $I_{P_{ij}}^{a,b}$, $I_{Q_{ij}}^{a,b}$ are the 2nd-order approximations of integrals, which are expressed as

$$I_{P_{ij}}^{a,b} = (a-b)\Delta t \delta_{P_{ij}}^{a,b} \overline{\mu}_{P_{ij}}^{a,b} H_j^k, \quad I_{Q_{ij}}^{a,b} = (a-b)\Delta t \delta_{Q_{ij}}^{a,b} \overline{\mu}_{Q_{ij}}^{a,b} H_j^k$$

$$H_j^k = H(P_{1j}^k, \cdots, P_{dj}^k, Q_{1j}^k, \cdots, Q_{dj}^k)$$

The notations δ and $\overline{\mu}$ denote difference quotient and mean difference operators.

IC/PP3042/025: A mortar finite elements for parabolic problems.

Presenter: Ajit Patel (IIT Bombay, India)
Co-author: Amiya Pani (IIT Bombay, India)
Co-author: Neela Nataraj (IIT Bombay, India)

In this paper, a mortar finite element method is used to discretize the space variable, a finite difference scheme is used for time discretization of the parabolic initial and boundary value problems. Optimal error estimates in L^2- and H^1-norms for both semidiscrete and fully discrete schemes are discussed. Numerical experiments are conducted to support the theoretical results.

IC/PP4343/025: Numerical simulation of dislocation dynamics.

Presenter: Petr Pauš (Czech Technical University, Prague, Czech Republic)

Dislocation dynamics is described by the mean curvature flow $v_\Gamma = -\kappa_\Gamma + F$. This law is treated uaing a parametric description. This evolution law is numerically solved by means of either the method of lines or an implicit scheme. Several numerical studies were performed in order to investigate properties of the above mentioned schemes, namely numerical convergence. Additionally we present several qualitative numerical computations showing behavior of dislocations under external stress field.

IC/PP3388/026: Numerical method for elliptic multiscale problems.

Presenter: Isabelle Greff (Universite de Pau et des Pays de l'Adour, France)

A large class of multiscale problems are described by partial differential equations with highly oscillatory coefficients. Such coefficients represent the properties of a composite material or the heterogeneity of the medium in the computation of flow in porous media problem. The computation of an accurate discrete solution of such problems requires a very fine discretisation associated with a fine grid $\mathcal{T}_h$. For such a fine resolution, the storage and computation costs are very high. From an engineer's perspective, we are interested in the average behaviour of the elliptic oscillatory operator on a coarse scale taking into account the small scale features without fully resolving them. We intend to provide a smoother elliptic operator which on a coarse mesh behaves like the original operator.

As a model problem, let us consider the elliptic boundary value problem on Ω, a bounded Lipschitz domain in $\mathbb{R}^d$, $Lu = f$ in Ω and $u = 0$ on $\partial\Omega$, with the right-hand side f in $L^2(\Omega)$. As an example, let

$$L = -\sum_{i,j=1}^{d} \frac{\partial}{\partial_j} \alpha_{ij} \frac{\partial}{\partial_i},$$

whose coefficients may be non-smooth; e.g., $\alpha_{ij} \in L^\infty(\Omega)$ is an oscillatory or jumping coefficient. We require certain real numbers $\underline{\lambda}, \overline{\lambda} > 0$ such that the matrix function $\alpha(x) = (\alpha_{ij})_{i,j=1,\dots,d}$ satisfies $0 < \underline{\lambda} \leq \lambda(\alpha(x)) \leq \overline{\lambda}$ for all eigenvalues $\lambda(\alpha(x))$ of $\alpha(x)$ and almost all $x \in \Omega$. Note that there is no requirement on smoothness or periodicity of the coefficients. Our goal is to construct an elliptic operator A with slowly varying coefficients which behaves similarly to the operator L on a coarse grid. To build A, we will consider the prolongation and restriction operators issued from the multi-grid method framework, and combine them with L. In the case of a T-periodic coefficient α, the homogenisation theory should provide a good operator [1]. To simplify the theory and the numerical implementations, we restrict ourselves to the one-dimensional case. Numerical results for different types of coefficient α (periodic or not) demonstrate the choice of the operator A we built.

This is joint work with Prof. Wolfgang Hackbusch (MPI, Leipzig).

[1] Bensoussan, A., Lions, J-L. and Papanicolaou, G.; *Asymptotic analysis for periodic structures*. North-Holland Publishing Co., 1978.

IC/PP739/026: The finite-element method on domains with conical or angular points.

Presenter: Hengguang Li (Department of Mathematics, the Pennsylvania State, USA)

Let Ω be either a polygonal domian in 2-D or a polyhedron in 3-D. Consider the Poisson's equation on Ω with the Dirichlet boundary condition: $-\Delta u = f$ in Ω, $u|_{\partial\Omega} = 0$. We shall show the well-posedness and regularity results for the solution u in some weighted Sobolev space $K_a^m(\Omega)$. In particular, we claim that there is no loss of K_a^m-regularity for the solution of the equation. We then provide an explicit construction of a sequence of finite dimensional subspaces V_n for the finite element method, such that the optimal convergence rate is attained for $u_n \in V_n$, i.e., $||u - u_n||_{H^1(\Omega)} \leq C\dim(V_n)^{-\frac{m}{2}}||f||_{H^{m-1}(\Omega)}$, with C independent of f and n. To be more precise, special meshes for vertices of a polygon or a polyhedron, and the meshes for edges of a polyhedron will be designed to overcome the pollution effects from the sigularities of the solution in the finite element method. Numerical results will be shown to verify our theoretical prediction. This method can extend to more general elliptic equations on domains with conical or angular points.

IC/PP4705/027: Error control in approximation of PDEs via topological gradient and hierarchical error estimator.

Presenter: Zoubida Mghazli (Université Ibn Tofail – Kenitra, Morocco)
Co-author: Abdellah Alla (Université Ibn Tofail – Kenitra, Morocco)
Co-author: Mohamed Masmoudi (Université Paul Sabatier Toulouse III, France)

The mesh adaptation is now an indispensable tool in engineering and simulation. The *a posteriori* error estimates and their use for mesh adaptation have become one of the principal axes of development in the numerical analysis of partial differential equations (PDE). The early a posteriori error estimates has been developed by I. Bubuska and W.C. Rheinboldt in 1978, and a large spectrum of this type of estimates has been devised, essentially for the Finite Element Methods (FEM) of elliptic problems. The main result consists of exhibiting local error indicators which can be computed explicitly as a function of the discrete solution and the data.

Within the FEM, various strategies of a posteriori error estimation have been derived during the last decades. The hierarchical methods are based on a simple idea: given an approximation of order k, a better approximation of order $k+1$ could be used to assess the accuracy of the solution. One only computes the defect-correction in higher order finite element. This gives, in the energy norm, global *a posteriori* error estimation on the solution of the PDE.

The aim of this presentation is to derive a method to control the error in an integral output functional of interest by using an adjoint-based hierarchical error estimation and mesh adaptation. Our approach is based on computing, via the asymptotic expansion, the topological gradient of an auxiliary functional depending on the primal and the dual hierarchical error estimator of the solution of PDE. We prove that this functional is equivalence to the error in functional of interest. The topological gradient is used as a criterion in the strategy of adaptation. Some numerical experiments, will be presented

03: Nonlinear Analysis and Dynamical Systems, Minisymposia

IC/MP270/015: Computational topology and dynamics.

Organiser: William Kalies (Florida Atlantic University, USA)
Co-organiser: Thomas Wanner (George Mason University, USA)

In recent years, computational topological methods have spurred the development of a class of numerical techniques for the rigorous, qualitative analysis of dynamical systems. These methods can provide rigorous verification for the continuation of equilibria, the detection of uniform hyperbolicity, the global decomposition of dynamical systems, and the existence of low dimensional dynamical structures such as fixed points, periodic orbits, connecting orbits, and chaotic dynamics. These methods have been applied to continuous maps such as the infinite-dimensional Kot–Schaffer map, the Swift–Hohenberg and Cahn–Hilliard partial differential equations, and other maps and differential equations. Central to these techniques are the Conley index and computational topology, in particular homology. Computational homology algorithms have also been used to study the dynamics of patterns generated by partial differential equations directly. These techniques have been applied to spinodal decomposition and coarsening in the Cahn–Hilliard equation and to characterize spatial-temporal chaotic behavior in the FitzHugh–Nagumo equations and experimental data of Rayleigh–Benard convection. This minisymposium covers a broad spectrum of computational topological methods including their implementation and their application to the study of dynamical systems.

Algorithms for symbolic dynamics and entropy bounds. **Sarah Day** (College of William and Mary, USA), Rafael Frongillo (Cornell University, USA), Rodrigo Trevino (University of Texas at Austin, USA) IC/MT1634/015

With recent advances in computing power, numerical studies of nonlinear dynamical systems have become increasing more popular. However, errors inherent to such studies may obscure the dynamics or, in the very least, raise doubts about the existence of numerically observed structures. Furthermore, unstable behavior, an intrinsic element of complicated systems, may be difficult to track even with very careful numerical work. I will discuss topological techniques which allow for the rigorous detection of dynamical structures of various stability types. In particular, I will focus on recent work on expanding these techniques that led to the computation of a rigorous lower bound on the topological entropy (one measurement of complexity) for the (chaotic) Henon map.

Computational aspects of Morse decompositions via algebraic lattices. **Robert Vandervorst** (Vrije Universiteit Amsterdam, The Netherlands), William Kalies (Florida Atlantic University, USA) IC/MT3073/015

We discuss the link between basic algebraic structures such as distributive lattices and Morse decompositions. Lattice theory provides simple algorithmic proofs for finding index filtrations and Lyapunov functions.

Computational approach to the Misiurewicz–Mañé theorem. **Hiroshi Kokubu** (Kyoto University, Japan) IC/MT2593/015

Uniform expansion outside a neighborhood of critical points of an interval map, which is known as the Misiurewicz and Mañé's theorem, is a crucial property for the study of one-dimensional dynamics. We shall discuss how this can be obtained, in the case of the quadratic maps, by a rigorous computational method using some graph algorithms. This work is done in collaboration with Sarah Day, Stefano Luzzatto, Konstantin Mischaikow, Hiroe Oka and Pawel Pilarczyk.

Building a data-base for the global dynamics of multi-parameter systems. **Konstantin Mischaikow** (Rutgers University, USA) IC/MT1635/015

It is well accepted that nonlinear dynamical systems can exhibit a wide variety of complex dynamics that may be sensitive to changes in parameters. It is also quite common in applications that not all values of the parameters have been determined. We outline a proposed method for building a data base that can be queried to determine parameter values at which particular types of dynamical structures can be found or values at which specific types of bifurcations occur. The fundamental idea is to use topological methods that are computationally efficient to store essential features of the dynamics in terms of a directed graph with equivalence classes of homology maps at the nodes. The directed graph represents information about the existence of a global Lyapunov function and the homology maps at the nodes encode information about the recurrent dynamics.

We explain these ideas in the context of a density dependent Leslie model arising from population biology.

IC/MP270/015: Computational topology and dynamics. #2

Organiser: William Kalies (Florida Atlantic University, USA)
Co-organiser: Thomas Wanner (George Mason University, USA)

(For abstract, see session #1 above.)

Homology algorithms and applications. **Marian Mrozek** (Jagiellonian University, Poland) IC/MT1193/015

Classical homology algorithms, based on the Smith diagonalization algorithm, are supercubical and therefore their applicability is very limited. We present some new ideas for homology algorithms based on one space homology theory and coreduction methods. The ideas lead to fast algorithms for cubical and simplicial homology and homology of maps. Working implementations of these algorithms will be presented and compared with other available algorithms. In the second part of the talk some applications to rigorous numerics of dynamical systems and differential equations as well as medical image analysis will be presented.

Uncertainty quantification for homology computations. **Thomas Wanner** (George Mason University, USA) IC/MT4963/015

Many partial differential equation models arising in applications generate complex time-evolving patterns which are hard to quantify due to the lack of any underlying regular structure. Such models may include some element of stochasticity which leads to variations in the detail structure of the patterns and forces one to concentrate on rougher common geometric features. In many of these instances, such as for example in phase-field type models in materials science, one is interested

in the geometry of sublevel sets of a function in terms of their topology, in particular, their homology.

Recent computational advances make it possible to compute the homology of discrete structures efficiently and fast. Such methods can be applied to the above situation if the sublevel sets of interest are approximated using an underlying discretization of the considered partial differential equation. Yet, this method immediately raises the question of the accuracy of the resulting homology computation.

In this talk, I will present a probabilistic approach which gives insight into the suitability of the above method in the context of random fields. We will obtain explicit probability estimates for the correctness of the homology computations, which in turn yield a-priori bounds for the suitability of certain grid sizes. In addition, we present a computational approach to homology validation in the above setting, and apply our results to certain stochastic partial differential equations arising in materials science.

Rigorous continuation of equilibria of PDEs defined on rectangular spatial domains. **Jean-Philippe Lessard** (Georgia Institute of Technology, USA), Sarah Day (College of William and Mary, USA), Marcio Gameiro (Rutgers University, USA), Konstantin Mischaikow (Rutgers University, USA) IC/MT1628/015

One of the most efficient methods for determining the equilibria of a continuous parameterized family of differential equations is to use predictor-corrector continuation techniques. In the case of partial differential equations this procedure must be applied to some finite dimensional approximation which of course raises the question of the validity of the output. We introduce a new technique that combines the information obtained from the predictor-corrector steps with ideas from rigorous computations and verifies that the numerically produced equilibrium for the finite dimensional system can be used to explicitly define a set which contains a unique equilibrium for the infinite dimensional partial differential equation. In this talk, we'll discuss about some work in progress regarding the above method applied on nonlinear PDEs defined on 2 dimensional rectangular domains.

Hyperbolicity, stability and monodromy of dynamical systems. **Zin Arai** (Kyoto University, Japan) IC/MT2608/015

In this talk, we propose a rigorous computational method for proving uniform hyperbolicity of given dynamical systems.

In general, the uniform hyperbolicity of the chain recurrent set implies the structural stability of the chain recurrent set, and then the structural stability enables us to construct a monodromy homomorphism from the fundamental group of the set of hyperbolic parameter values to the automorphism group of the symbolic dynamics that describes the chain recurrent set of the given system. By computing the monodromy homomorphism, we can reveal the structure of the parameter space of the given dynamical system.

We also present examples of application of the method which include real and complex Hénon maps, and the nonlinear Leslie population model.

IC/MP52/033: On fractional calculus and its applications.

Organiser: Mokhtar Kirane (Université de La Rochelle, France)
Co-organiser: Juan Trujillo (Universidad de La Laguna, Spain)

During the last years, fractional differential equations have assumed an important role in modelling the anomalous dynamics of numerous processes related to complex systems in a large number of diverse areas of science and engineering: Physical Chemistry (sub- and super-diffusion), Geophysics, Materials Theory, Financial Engineering (fractional Black–Scholes Equations), Biology, Signal Processing, Fractional Motion Control, Plasma Physics, etc. This minisymposium is intended to offer some selected methods applied to some representative equations/systems. The presented topics include: nonlinear reaction diffusion equations with fractional powers of the Laplacian, nonlinear diffusion, equations with time fractional derivatives, wave equations with damping of fractional order, fractal equations in quantum mechanics, fractal Burgers' equation, numerical analysis of fractional differential equations.

Activities: a round table on this emergent field will be organized. Future research directions will be discussed.

Fractional equations from fractional variations. **Vasily Tarasov** (Moscow State University, Russian Federation) IC/MT372/033

Fractional generalization of an exterior derivative for calculus of variations is defined. Fractional equations of motion are obtained by fractional variation of Lagrangian and Hamiltonian that have only integer derivatives. Fractional generalization of Hamiltonian and gradient systems are considered by using differential forms and exterior derivatives of noninteger orders.

Fractional variational principles and their applications. **Dumitru Baleanu** (Cankaya Universitesi, Turkey) IC/MT380/033

Variational calculus and Fractional Calculus have played a significant role in various areas of applied sciences such as, among others, Physics, Engineering and Economics. This topic is deeply connected to the very recent developments in theoretical aspects and especially in the numerical schemes of fractional differential equations. In the first part of my talk the fractional Lagrangian formalisms are analyzed, whereas in the second part the fractional Hamiltonian formalisms are discussed. I will expose in this talk the fractional generalization of the traditional variational principles to the constrained systems for both discrete and continuous cases. Also I will present several illustrative examples of fractional Euler-Lagrange and Hamilton equations admitting both analytical and numerical solutions.

Fractional differential equations: interpretations of fractional-order operators and initial conditions in terms of fractional derivatives. **Igor Podlubny** (Kosice, Slovakia) IC/MT377/033

Fractional integration and fractional differentiation are generalisations of notions of integer-order integration and differentiation, and include n-th derivatives and n-folded integrals (n denotes an integer number) as particular cases. Because of this, it would be ideal to have such physical and geometric interpretations of fractional-order operators, which will provide also a link to known classical interpretations of integer-order differentiation and integration.

For proper use in applications, having some interpretations only for fractional order operators is not sufficient. Indeed, there is also a need to understand the meaning of initial conditions for fractional differential equations. Such initial conditions, in general, are expressed as limit values of fractional derivatives and/or integrals.

In our presentation based on our recent investigations we will present interpretations for the fractional order operators and

for the initial conditions expressed in terms of such operators.

First, we will discuss and illustrate several approaches to geometric and physical interpretations of fractional order operators, which appear in fractional differential equations. Then we will demonstrate that it is possible to attribute physical meaning to initial conditions expressed in terms of Riemann-Liouville fractional derivatives, and that it is possible to obtain initial values for such initial conditions by appropriate measurements or observations.

Fractal Hamilton–Jacobi–KPZ equations. **Wojbor Woyczynski** (Case Western Reserve University, USA) IC/MT381/033

Nonlinear and non-local evolution equations of the form $u_t = Lu \pm |\nabla u|^q$, where L is a pseudo-differential operator representing the infinitesimal generator of a Lévy stochastic process, have been derived as models for growing interfaces in the case when the continuous Brownian diffusion surface transport is augmented by a random hopping mechanism. The goal of this paper is to study properties of solutions to this equation resulting from the interplay between the strengths of the *diffusive* linear and *hyperbolic* nonlinear terms, posed in the whole space $\mathbb{R}^N$, and supplemented with non-negative, bounded, and sufficiently regular initial conditions.

This is joint work with Greg Karch.

IC/MP52/033: On fractional calculus and its applications. #2

Organiser: Mokhtar Kirane (Université de La Rochelle, France)
Co-organiser: Juan Trujillo (Universidad de La Laguna, Spain)

(For abstract, see session #1 above.)

On the fractional telegraph problem. **Nasser eddine Tatar** (King Fahd University, Saudi Arabia) IC/MT402/033

In this talk we shall be concerned with the fractional telegraph problem. This problem arises while studying some iterated Brownian motions. The equation involved can be looked at as a generalization of the weakly internally damped wave equation. The first (corresponding to the weak internal damping) and the second order temporal derivatives are replaced by fractional derivatives. The questions of well-posedness, stability and blow up in finite time will be addressed. Some new methods and techniques will be presented. Moreover, several interesting special cases will be highlighted.

Finite-time blow-up and life span of a non-automomous semilinear equation. **Aroldo Perez-Perez** (Universidad Juárez Autónoma de Tabasco, Mexico) IC/MT400/033

Consider the semilinear nonautonomous equation $\frac{\partial}{\partial t}u(t) = k(t)\Delta_\alpha u(t) + u^{1+\beta}(t)$ with $u(0,x) = \lambda\varphi(x)$, $x \in \mathbb{R}^d$, where $\Delta_\alpha := -(-\Delta)^{\alpha/2}$, $0 < \alpha \le 2$, $\lambda, \beta > 0$ are constants, $\varphi \ge 0$ is bounded, continuous and does not identically vanish, and $k : [0,\infty) \to [0,\infty)$ is a locally integrable function satisfying $\varepsilon_1 t^\rho \le \int_0^t k(r)\,dr \le \varepsilon_2 t^\rho$ for all t large enough, where $\varepsilon_1, \varepsilon_2, \rho > 0$ are given constants. We prove that any constellation of positive parameters d, α, ρ, β, obeying $0 < d\rho\beta/\alpha < 1$, yields finite time blow up of any nontrivial positive solution. Under suitable additional assumptions, we also obtain upper and lower bounds for the life span $T_{\lambda\varphi}$ of the above equation, which prove that $T_{\lambda\varphi} \sim \lambda^{-\frac{\alpha\beta}{\alpha - d\rho\beta}}$ near zero. "Work done in collaboration with Kolkovska, E.T. and López-Mimbela, J.A".

Diffusion-wave and relaxation problem. **Mirjana Stojanovic** (Univerzitet u Novum Sadu, Yugoslavia) IC/MT383/033

By the notion of fractional derivative of distributed order we consider the time fractional equation of distributed order

$$\int_0^2 p(\beta)[D_*^\beta u(t,\cdot)]d\beta = \rho^2 \frac{\partial^2}{\partial x^2}u(t,\cdot),\ p(\beta) > 0, \qquad (1)$$

where $p(\beta)$ is the weighted function, $x \in \mathbf{R}$, $t \ge 0$, subject to the initial data $u(0^+,\cdot) = \varphi(\cdot)$, $u_t(0^+,\cdot) = \psi(\cdot)$, D^β concerns the Caputo derivative.

As method for construction of the solution we use in sequence Fourier and Laplace transform and their inverse.

We prove the existence-uniqueness of the solution and regularity of the solution in the space $C^\infty(\mathbf{R})$, (w.r.) to the spatial variable, when the initial data are L^2-functions. We find upper viscosity solutions.

We generalize result to two-term, three-term and finally n-term equation.

This equation have an application in visco-elasticity and in anomalous diffusion processes.

Concerning the investigation of the diffusion-wave problem, we conclude the following: for $\beta = 1$ we have heat equation which smooths all the rough, singular initial data. For $\beta = 2$ we have wave equation which propagate singularities of the initial data. Diffusion-wave equation ($0 < \beta < 2$,) gives as a solution C^∞-function (w.r.) to the spatial variable x if the initial data are bounded in L^2-norm. Thus, the operator of the diffusion-wave equation have more properties of heat operator. It smoothes initial data, but requires their boundedeness in L^2-norm.

We consider fractional relaxation equation of distributed order in interval $(0,2)$ using Caputo derivatives approach:

$$\int_0^2 p(\beta)D_*^\beta u_*(t)dt = -\lambda u_*(t) \qquad (2)$$

subject to he initial data $u(0_*^+) = 1$, where $p(\beta) \ge 0$, $\int_0^1 p(\beta) = P > 0$. Constant P can be normalized to 1, $*$ is the sign for Caputo derivative.

We find exact solution using different weighted functions giving solutions in intervals $(1,2)$ and $(0,2)$. We give the qualitative analysis of the solutions, their asymptotic behavior at zero and infinity. For behavior between the extremals we use integral representation of the solution and prove the oscillatory character finding the number of zeros of the solution in interval $t \in [0,\infty)$.

The solution of the relaxation equation on interval $(0,2)$ inherits the asymptotic behavior of the solution on the interval $(0,1)$. In the interval $(0,1)$ the solution have the relaxation properties, tends to zero as $t \to \infty$, while in the interval $(0,2)$ the solution oscillate.

Adaptive quadratures and fractional IDEs: applications in image processing. **Eduardo Cuesta** (Universidad de Valladolid, Spain) IC/MT364/033

In this work we consider partial integro-differential equations of fractional order whose prototype is

$$(1)\quad u(t,x,y) = u_0 + \int_0^t \frac{(t-s)^{\alpha-1}}{\Gamma(\alpha)}\Delta u(s,x,y)\,ds + f(t,x,y), \quad (t,x,y) \in [0,T]$$

where $1 < \alpha < 2$, $\Omega \subset \mathbb{R}^2$ and Δ stands for the 2-D Laplacian.

Numerical schemes to approximate the solution of (1) have been widely studied in literature, in particular the ones based on fractional convolution quadratures. However, the high com-

putational cost of these methods made its use in practical applications unaffordable the most of times. Therefore, it is not surprising that the effort of many authors concentrates at present not only in finding higher order numerical methods but in obtaining faster and more efficient algorithms.

In this way, our main contribution consists in the obtention of adaptive time discretizations which will allow us to keep the error under a given tolerance thanks to a suitable choice of the step setting and, of course, with a noticeable computational cost reduction.

Numerical experiments will be provided, in particular some involving image processing and filtering where the computational cost is a crucial drawback.

IC/MP88/033: Bifurcation analysis in experiments.

Organiser: Yuliya Kyrychko (University of Bristol, UK)
Co-organiser: Jan Sieber (University of Aberdeen, UK)

The aim of the minisymposium is to present and dicuss methods for the analysis and tracking of bifurcations directly in real-life experiments. The requirement of feasibility in an experiment, which these methods have to satisfy, is fundamentally different from the well-researched numerical efficiency. We aim to bring together experts who have approached this challenging problem from different angles and in various contexts. The approaches we plan to present range from feedback control based on linear system identification or time series analysis to equation-free methodologies, which have been successfully applied to computational black-box simulators.

Bifurcations in impact oscillators. **Celso Grebogi** (University of Aberdeen, UK) IC/MT1692/033

A system is an impact oscillator if it has an oscillating object that impacts frequently with some other object. Impact oscillators occur in many technological situations. For example, mechanical devices are often engineered with loose fitting joints to accommodate thermal expansion, and the dynamical behaviour of such systems often leads to impacts in the joint. In addition, many machines inevitably suffer from effects of vibro-impacts. A common feature shared by models of these systems is the smoothness of the systems between the impacts. In this talk, I will use a simple physical system as a prototype impact oscillator. A mass is attached to a linear spring that is fixed to a wall. There is sinusoidal external force acting on the mass. The friction force is proportional to the velocity of the mass. When the amplitude of oscillation is sufficiently small, there are no impacts between the mass and the wall, and the dynamics of the system is the same as that of a forced damped harmonic oscillator without the wall. As the amplitude of oscillation is increased, the mass begins to have impacts with the wall, first with very low velocity. The bordering state between the impacting and non-impacting is called a grazing impact, i.e., when the mass contacts with the wall with zero velocity. Interesting new bifurcations are observed at grazing, and they are called grazing bifurcations. Grazing bifurcations are important physical examples of a general type of bifurcation called "border-collision bifurcations". The purpose of this talk is to present an analysis of grazing bifurcations in impact oscillators. These bifurcations are "unconventional" in that they do not occur in smooth systems. The bifurcations presented in this talk are, however, expected to be universal for such systems and to apply to many systems in which impacts occur. I will also mention results on the control of impact oscillators when in a chaotic state.

Bifurcations in multi-section semiconductor lasers. **Hans-Jürgen Wünsche** (Humboldt-Universität zu Berlin, Germany), Oleg Ushakov (Humboldt-Universität zu Berlin, Germany), Sylvia Schikora (Humboldt-Universität zu Berlin, Germany), Fritz Henneberger (Humboldt-Universität zu Berlin, Germany) IC/MT2332/033

Multi-section semiconductor lasers represent a new class of optical devices. Their complex dynamics makes them promising candidates for applications in optical communication networks. We summarize experiments with lasers consisting of three individually contacted sections. In the parameter space of the three easily tunable injection currents, they exhibit a rich variety of operational modes. Among them are continuous-wave operation, regular power pulsation, and also chaotic emission. Due to the extremely short time scales between nanoseconds and picoseconds, the underlying bifurcations can be identified only from measured optical and power spectra. To these purposes, the response to external perturbations is used as additional fingerprint of the type of a bifurcation. Examples are the decreasing line width of noise-induced precursurs of Hopf bifurcations and the extremely long chaotic transients upon pulsed excitation close to a boundary crisis. The unstable states born in bifurcations play an important role but usually they are not accessible in experiment because visited at most for short times only. To overcome this difficulty, we have developed an all-optical version of noninvasive time-delayed feedback control. Optical feedback from an external Fabry-Perot resonator is exploited. Path-following of unstable steady and pulsating states beyond Hopf and period doubling bifurcations, respectively, is demonstrated with this method. The experimental results will be supplemented by numerical simulations and a bifurcation analysis of the underlying model equations.

Model-based experimental bifurcation analysis. **Ulrich Parlitz** (Universität Göttingen, Germany), David Engster (Universität Göttingen, Germany), Jörg Dittmar (Universität Göttingen, Germany) IC/MT2257/033

Different modelling methods are employed to predict and track bifurcation points in experimental systems using a few measured time series, only. If no physical model of the underlying process is available black-box models have to be generated from the data which are able to reproduce the observed longterm dynamics including proper parameter dependence. We shall present criteria and strategies for providing such models and practical examples illustrating their performance.

Bifurcations in power electronic converters. **Stephen Hogan** (University of Bristol, UK) IC/MT2769/033

In many control problems, the control strategy is phrased in terms of average quantities. In this paper we prove the general result that, given a linear system $\dot{x} = Ax + u$ where A is hyperbolic, u is piecewise linear and L-periodic, such that $\int_0^L u(t)dt = 0$, then there exists a unique L-periodic solution $x = x_p(t)$ such that $\int_0^L x_p(t)dt = 0$. We then consider a DC/DC buck (step-down) converter controlled by the ZAD (zero-average dynamics) strategy. The ZAD strategy sets the *duty cycle*, d (the length of time the input voltage is applied across an inductance), by ensuring that, on average, a function of the state variables is always zero. The two control parameters are v_{ref}, a reference voltage that the circuit is required to follow, and k_s, a time constant which controls the approach to

the zero average. We show how to calculate d exactly for a periodic system response, without knowledge of the state space solutions. In particular we show that for a T-periodic response d is *independent* of k_s. We calculate curves in (v_{ref}, k_s) space at which a T-periodic response of the system undergoes period doubling and corner collision bifurcations, the latter occurring when the duty cycle saturates and is unable to switch. We also show the presence of a codimension two bifurcation in this system when a corner collision bifurcation and a saddle node bifurcation collide, to produce stable unsaturated $2T$-periodic responses which can be obtained either in the presence or absence of the stable T-periodic response.

Work done in collaboration with E. Fossas and T. M. Seara (Universitat Politècnica de Catalunya, Barcelona, Spain)

IC/MP88/033: Bifurcation analysis in experiments. #2

Organiser: Yuliya Kyrychko (University of Bristol, UK)
Co-organiser: Jan Sieber (University of Aberdeen, UK)

(For abstract, see session #1 above.)

Design of computational experiments for bifurcation computations. **Yannis Kevrekidis** (Princeton University, USA) IC/MT3032/033

We will discuss equation-free computation as a protocol for design of computational experiments. In particular, we will study cases where the goal of the coarse-grained computation is the location of coarse bifurcation points.

Bifurcations in a spring–pendulum oscillator. **Alicia Gonzalez-Buelga** (University of Bristol, UK), Yuliya Kyrychko (University of Bristol, UK), David Wagg (University of Bristol, UK) IC/MT1161/033

In this paper we study experimentally the dynamics of a non linear system: a spring pendulum coupled to an oscillator. The system was tested using a hybrid technique called Real Time Dynamic Substructuring (RTDS). RTDS is a testing technique that involves splitting the system under study into two subsystems: one will be physically tested (physical substructure) and the other will be simulated in the computer (numerical model). Typically the numerical model is a linear well known behaviour subsystem while the substructure is a nonlinear unknown dynamics subsystem. These substructures interact in real time trough a set of transfer systems.

RTDS is a very powerful experimental methodology that not only allows full scale and real time testing but also real-time bifurcation tracking in complex engineering systems. The fact that part of the system is represented by its numerical model permits manipulation of the systemŠs characteristics in real-time.

In our hybrid experiment the spring pendulum is taken to be the tested physical substructure while oscillator is the simulated numerical model. This presentation focuses on experimental study of single and multi-parameter bifurcations. These studies are not possible from a full physical experiment and show the possibilities of using a hybrid numerical-physical technique.

Global properties of time-delayed feedback control with unstable control loop in electronic circuit experiments. **Klaus Höhne** (TU Darmstadt, Germany) IC/MT2504/033

Time-delayed feedback control is an efficient tool, both in theory and experiment, to stabilize unstable periodic orbits embedded in a chaotic attractor. One of the most important restrictions of this method arises from the so-called odd-number-limitation, i.e. torsionfree unstable periodic orbits cannot be stabilized by conventional time-delayed feedback control. Here we report on experiments in an electronic unstable van der Pol oscillator. We succeeded in controlling a torsionfree unstable periodic orbit by applying the method of an unstable time-delayed feedback controller. Our investigations showed that control often fails due to a small basin of attraction. We found, however, that the global control performance can dramatically be improved by varying the coupling between the system and the control loop. Our experimental findings are consistent with considerations from bifurcation theory and in very good agreement with numerical simulations.

Nonlinear modal interactions and model reduction of a kicked flexible rod. **Joseph Cusumano** (Pennsylvania State University, USA) IC/MT2795/033

We present a detailed experimental study of the dynamics of a flexible steel rod kicked by a spatially triggered electromagnet. This nonlinear oscillator provides an excellent model problem with which to study empirically-assisted methods for generating low-order models from infinite-dimensional dynamical systems.For all values of the kicker magnet voltage V, motions starting with sufficiently small initial conditions asymptotically approach the stable trivial solution of the system. However, above a critical voltage, a bifurcation occurs giving rise to a stable/unstable limit cycle pair. As V increases, spectral bifurcation diagrams show four distinct dynamical regimes: small amplitude limit cycle; quasiperiodic response; chaos; and large amplitude limit cycle. The Proper Orthogonal Decomposition (POD) is used to study the effective dimensionality and modal interactions in the system. It is shown that two specific nonlinear modes dominate in the observed dynamics over the entire range of the kicker voltage, and hence it might reasonably be expected that a two degree of freedom (DOF) model is adequate to describe the observed behavior. Phase space reconstruction of time series data and nonlinear prediction provide an independent confirmation of this effective dimensionality. Motivated by these experimental results, a simple 2 DOF model is developed. It is shown that the model provides a good qualitative match to the experimental system, including both the modal and bifurcation structures. We conclude by discussing some of the difficulties and outstanding research questions in using POD for such model reductions.

IC/MP245/033: Dynamical systems with cosymmetry: numerics, bifurcations, applications.

Organiser: Vyacheslav Tsybulin (Rostov State University, Russian Federation)

A new object in cosymmetrical systems is a family of steady states with variable spectra. This case is the opposite of the symmetry situation when all the states have identical spectrum. It is very interesting to consider the effects produced by the appearance of such a continuous family. Now the non-trivial bifurcations were found in cosymmetrical problems: the delay with limit cycle branching off, new scenario of tori birth etc. The investigation of all these problems has required the development of new numerical methods and the study of approaches in the bifurcation theory of dynamical systems. The

proposed talks will present recent results on the cosymmetry theme. Partially, we plan to consider: Evolution of steady states family in 2d and 3d convection in a porous medium, cosymmetrical effects in some population kinetics problems, numerical approaches to computation of steady states family, special cosymmetrical bifurcations, computer experiment on the selection of steady states from the continuous family.

The co-symmetric bifurcations in the planar filtrational convection problem: numerical results. **Vasily Govorukhin** (Rostov State University, Russian Federation) IC/MT870/033

Theory of cosymmetry was introduced by Yudovich [1] to explain a phenomenon of existence of one-parameter family of stationary flows in the planar filtrational convection problem. It was shown that the branching of cycle of equilibria (CE) is a typical bifurcation in cosymmetric dynamical system [1]. In [2] and in many other works of these authors the theory of cosymmetric bifurcations was developed.

We investigate the planar filtrational convection problem in rectangular container numerically by Galerkin method. We consider Galerkin systems of various dimensions (up to 1000) and we study numerically the bifurcations connected mainly with CE existence.

The bifurcations of CE was found out: birth of a new family from already existing, intersection and join of CE, origin of a CE Šfrom an airŠ etc [3-4]. The bifurcations of families are connected with different CE both with stable and with unstable. The periodic, quasiperiodic and chaotic regimes were founded for different values of parameters [4]. The steady periodic regimes can occur by two ways: as a result of cosymmetric Hopf or Euler bifurcations. For some values of parameter transition from stationary movement at once to chaotic ones is possible. The bifurcation of tori branching from CE was found.

The qualitative repetition of bifurcation and consistency of bifurcation parameter values was established by different dimensions Galerkin's models investigation. We found practically all types of bifurcations studied theoretically in [2].

[1] Yudovich V.I. Matem. Zametki 49, 1991; Chaos 5 (2), 1995.

[2] Kurakin L.G. and Yudovich V.I. Chaos 10 (2), 2000; Chaos 11 (4), 2001.

[3] Govorukhin V.N. Fluid Dynamics, V. 34, No. 5, 1999.

[4] Govorukhin V.N., Shevchenko I.V., Fluid Dynamics, V. 38, No. 5, 2003; V. 41, No. 6, 2006.

Co-symmetric families of steady states in 3D convection of the incompressible fluid in a porous medium. **Vyacheslav Tsybulin** (Rostov State University, Russian Federation) IC/MT884/033

Three-dimensional convection of the incompressible fluid in a porous medium is considered. Mimetic finite-difference schemes for the primitive variables equation are developed. The connection of a derived staggered discretization with a finite-difference approach based on the stream function (planar problem) is established. Continuous cosymmetric families of steady states are computed and stability analysis is presented.

Selection of steady states in planar Darcy convection. **Bülent Karaözen** (Middle East Technical University, Turkey), Vyacheslav Tsybulin (Rostov State University, Russian Federation) IC/MT1732/033

Selection of steady states in the planar convection problem for the incompressible fluid in a porous medium is studied. The perturbation of initial data by adding of the harmonic deviation of boundary temperature is analyzed. Computer experiments on the selection of equilibria show that, for initial distribution (disturbance) with large amplitude, the neighborhood of a single preferable steady state is established. The question is why some patterns of fluid are more preferred than others. This problem is may be treated as a some variant of the description of separation processes. Important future problem here is a possibility to control the pattern organization.

Dynamics and family of equilibria in a population kinetics model with cosymmetry. **Katya Kovaleva** (Rostov State University, Russian Federation), Kurt Frischmuth (Universität Rostock, Germany) IC/MT2658/033

This work continues the study have started in [1] with a system of nonlinear parabolic equations with cosymmetry. We assume three populations sharing a common space and suppose a dominant role of the unique spatial coordinate. Looking for best opportunities for their respective trades, each population may move in dependence on the current concentrations of their own kind and the other one. However, the first population (thrives on relocation of the others, while the second and third suffer from motion of the first. We use a finite-difference scheme preserving the cosymmetry property for a given problem. Two cases of boundary conditions are considered. Different scenarios of instability for the state of rest are observed. Numerical results on computation of continuous families of steady states and periodic regimes are presented and stability of the zero equilibrium are studied.

1. K. Frischmuth, V. Tsybulin, Families of equilibria and dynamics in a population kinetics model with cosymmetry, Physics Letters **A 338** (2005), 51–59.

IC/MP79/034: Pattern formation in coupled-cell systems.

Organiser: William Langford (University of Guelph, Canada)

Systems of coupled oscillators (or *cells*) occur in very diverse applications, ranging from animal gaits and neural networks to heat exchanger arrays. Earlier work focussed on systems with a high degree of symmetry, leading naturally to complex spatio-temporal patterns via equivariant Hopf bifurcation theory. Recent work includes more general architectures represented by directed graphs, and reveals new behaviors such as nilpotent bifurcations occurring in codimension one.

Synchrony in coupled systems and the vestibular system. **Martin Golubitsky** (University of Houston, USA) IC/MT3884/034

Synchrony and phase synchrony were first studied in coupled systems using network symmetry. More generally, robust synchrony in a network of identical subsystems (cells) follows from a combinatorial condition (balanced coloring) and robust phase synchrony corresponds to symmetry in quotient networks. We review this earlier work and discuss phase shift synchrony in the context of that part of the vestibular system which connects inner ear canal nerves with neck muscle motoneurons. This later work is joint with Ian Stewart and LieJune Shiau.

Coupled cell networks: minimality and quotients. **Manuela Aguiar** (Universidade do Porto, Portugal), Ana Dias (Universidade do Porto, Portugal), Martin Golubitsky (University of Houston, USA), Maria Leite (University of Purdue, USA), Ian Stewart (University of Warwick, UK) IC/MT3902/034

Non-isomorphic coupled cell networks can correspond to coupled-cell systems with equivalent dynamics and are called ODE-equivalent. Coupled cell systems restricted to flow-invariant subspaces defined by equality of certain cell coordinates correspond to quotient networks. In this talk we discuss some recent results related with ODE-equivalence of coupled cell networks, minimality of ODE-classes and quotients networks.

Stability computations for nilpotent Hopf bifurcations. **Maciej Krupa** (New Mexico State University, USA), Martin Golubitsky (University of Houston, USA) IC/MT3948/034

Nilpotent Hopf bifurcations can occur in codimension one in coupled cell systems. Elmhirst and Golubitsky studied such bifurcations and obtained rather unusual branching patterns. In this work we use normal form theory to obtain stability results for some of the branches found by Elmhirst and Golubitsky. On the way to obtaining our results we determine how some of the synchrony subspaces of the network influence the structure of the normal form.

Spatio-temporal patterns in heat-exchanger arrays. **William Langford** (University of Guelph, Canada) IC/MT3930/034

Flow-induced vibrations of the tubes in a large heat exchanger array can cause metal fatigue and failure, leading to costly repairs. A simple mathematical model is presented for the case of a rectangular array, so that the problem becomes a study of the spatio-temporal patterns in a two dimensional coupled cell system with $\mathbb{Z}_M \times \mathbb{Z}_N$ symmetry. The results presented here include all the generic equivariant Hopf bifurcations in this setting, with their onset, stability and spatio-temporal patterns, for cases with the spatial periodicities that are likely to occur, both with and without an internal $\mathbb{Z}_2$ symmetry. The predictions of this analysis are in good qualitative agreement with experiments on flow-induced vibrations in arrays of circular cylinders performed at Atomic Energy Canada Limited. This is joint work with R. Akila, Garyounis University, Benghazi, Libya.

IC/MP326/034: Symmetry aspects in biological dynamical systems.

Organiser: LieJune Shiau (University of Houston, USA)
Co-organiser: Marc Timme (Max-Planck-Institut Göttingen, Germany)

This minisymposium features novel results on models of various biological dynamics, with a focus on underlying symmetries and on breaking these symmetries. Topics range from mechanisms of muscle movements to pattern formation and non-standard dynamics in biological neural networks.

In particular, one study is about the principles of neck muscle movements in most vertebrates (including humans), based on the semicircular canal input from the ears in the vestibular (balancing) system. Two studies investigate heteroclinic networks and unstable attractors, arising naturally in networks of neural oscillators. These features lead to the phenomenon of switching between neural *encoding* states, with potential implications, among others, for odor recognition and processing in insects. Another one shows that the number density of singular points, called pinwheels, in cortical pattern forming systems follows a universal statistics, with its mean normalized density close to the mathematical constant π. A theoretical model of pattern formation in the cortex explains this result. Also, a new dynamical phenomenon is found and analyzed in the study of globally coupled neural networks. Here the dynamics shows the irregular and chaotic appearing in transients, although it is governed by negative Lyapunov exponents. A relation to *stable chaos* is also discussed.

All speakers will present the basics and symmetries of the biological systems studied, and discuss their results.

Heteroclinic networks and clustering in simple models of neural activity. **Gábor Orosz** (University of Exeter, UK), Peter Ashwin (University of Exeter, UK) IC/MT1991/034

The dynamics of neural systems has to balance seemingly contradictory requirements of robustness to noise and sensitivity to inputs. Networks of coupled systems can however deliver this in cases where they have attractors that are heteroclinic networks giving so-called 'winnerless competition' between unstable states. We consider some specific examples motivated by work on the insect antennal lobe that convert spatially dependent inputs into spatio-temporal codes, where one can verify robustness with high sensitivity to inputs.

Stability properties of the asynchronous regime in a network of identical neurons. **Antonio Politi** (Consiglio Nazionale delle Ricerche, Italy) IC/MT991/034

The stability of globally coupled neurons is usually carried out by following a mean field approach. With reference to a system of leaky-integrate-and-fire neurons, we develop a microscopic approach that allows for an exact stability analysis. As a result we find that the mean field approach does not always provide the correct answer. This is issue is connected to the noncommutativity of two limits: infinitely many neurons and delta-like pulses. We also discuss the occurrence of some bifurcations that break the time-invariance of the asynchronous regime and the effect of a small dilution (cutting some links) which may give rise to a linearly stable but irregular regime.

Symmetry and bifurcation in vestibular system. **LieJune Shiau** (University of Houston, USA), Martin Golubitsky (University of Houston, USA) IC/MT1485/034

The vestibular system in most vertebrates, particularly in humans, controls balance by six semicircular canals to detect angular accelerations of the head motion. Signals from the canals are transmitted to eight groups of neck motoneurons thus the eight corresponding muscle groups. Through symmetry architecture and coupled cell network, we show that there are six possible spatiotemporal time-periodic states that can arise by Hopf bifurcation from an equilibrium representing an immobile head. We interpret these patterns as motions of the head and note that all six types of pattern appear to correspond to natural head motions.

Linearly-unstable attractors: charge loss induces heteroclinic switching in spiking neural networks. **Marc Timme** (Max-Planck-Institut Göttingen, Germany) IC/MT1591/034

The brain processes information in networks of nerve cells (neurons) which interact by sending and receiving electrical pulses, called spikes. The response of a biological neuron to incoming signals strongly depends on whether or not it has just emitted a spike. Here we propose a simple model of coupled neurons with partial response to residual input charges after spike emission. We study their collective network dynamics in the regime where the individual neurons dynamics is oscillatory and the interactions are delayed. For concave rise functions the system exhibits heteroclinic switching between cluster states (saddle periodic orbits) for an open set of a charge-loss parameter. We show that the saddle periodic orbits become unstable attractors (linearly unstable periodic orbits that are attractors in the sense of Milnor) in the limit of complete charge-loss, where the system becomes non-invertible.

IC/MP326/034: Symmetry aspects in biological dynamical systems. #2

Organiser: LieJune Shiau (University of Houston, USA)
Co-organiser: Marc Timme (Max-Planck-Institut Göttingen, Germany)

(For abstract, see session #1 above.)

Symmetry in sympathy: speciation as pattern formation in phenotype space. **Toby Elmhirst** (University of British Columbia, Canada) IC/MT3419/034

It has long been debated whether dimorphism can arise in a monomorphic population in a homogeneous environment, or whether a species can only diversify if different populations are geographically isolated from each other. I will present a class of systems, known as "pod systems", that brings out the symmetry of this question, and shows that dimorphism can appear in a population through a symmetry-breaking bifurcation. Thus we can see the appearance of biological diversity as pattern formation in phenotype space.

The general approach is to view a population as a density distribution over phenotype space. A monomorphic population is thus seen as a unimodal distribution, and a dimorphic one is bimodal. The systems I will discuss allow us to view the dynamics of a distribution over a spatial domain in terms of an $\mathbf{S}_N$-equivariant system of ODEs. The action of $\mathbf{S}_N$ means that a fully symmetric solution is a unimodal distribution — a marked difference from the usual symmetry-breaking analysis of systems on a domain in which fully symmetric solutions are spatially homogeneous. Thus we are able to analyse symmetry-breaking bifurcations from unimodal distributions, and we find that at primary symmetry-breaking bifurcations there exists, generically, a unique branch of bimodal distributions.

A mathematical constant in the design of the visual cortex. **Fred Wolf** (Max-Planck-Institut Göttingen, Germany) IC/MT3021/034

In the cortex of the mammalian brain, visual information is processed by a complex 2-dimensional pattern of functional modules called the orientation preference map. Because in young animals this structure is thought to arise by a dynamics of neuronal development a central aim of current research is the identification of dynamical models that can reproduce its spatial organization. Recently, the introduction of biologically plausible symmetry principles has enabled the identification of promising candidate models of visual cortical circuit development.

To provide a firm basis for comparing experimental observations and the predictions of such models, we quantitatively characterized the spatial statistics of singular points, called pinwheel centers, in orientation preference maps in a wide variety of animal species including monkeys, carnivores, and shrews. These species have evolved separately for more than 50 million years, occupy different ecological niches, and exhibit distinct patterns of visual behavior. Surprisingly, we found that numerous statistics of singular points including their spatial density, their count variance, and the next neighbor distance distributions of singular points are quantitatively indistinguishable, i.e. universal in the species studied. Most suggestive of a mathematical structure underlying this universality, the mean non-dimensional spatial density of singular points turned out to be 3.14 ± 0.03 being statistically indistinguishable from a well known mathematical constant.

Theoretical analyzes show that the observed universal statistics are quantitatively reproduced by models of cortical self-organization exhibiting a recently introduced permutation symmetry if their behavior is dominated by long-range interactions. We conclude that the experimentally observed universal statistics are emergent signatures of a dominant role of long-range interactions in the self-organization of cortical neuronal circuits.

Critical branching processes in neural networks. **Anna Levina** (Universität Göttingen, Germany) IC/MT3918/034

Self-organized critical dynamics occurs in a variety of systems. Commonly the activity of such systems during avalanches is modeled by branching processes. Under certain circumstances, this approach is justified by the specific topology of the system. In the sandpile model, for instance, an active site can activate only lower lying neighbours and cyclic activation is impossible.

Recent experimental research gave evidence of critical avalanches generated by a system far more complicated than a sendpile: neuronal activity in slices of rat cortex and neuronal cultures exhibit critical avalanche dynamics in the propagation of spontaneous activity. To model these more complicated dynamics, for simplicity, also branching processes were used, although it is unclear whether these are an appropriate approximation even for highly recurrent networks.

Here we establish a direct correspondence between avalanches generated by a critical branching processes and by a fully connected network of integrate-and-fire neurons. Such networks has been shown to exhibit power-law avalanches distribution observed experimentally. We present strong evidence justifying use of the branching processes for simulation and analysis of recurrent neural networks.

The discovered correspondence leeds to the suggestion of the simple learning rule, which allows self-organization of the network towards critical state.

IC/MP279/034: Geometry, dynamics, and control.

Organiser: Dmitry Zenkov (North Carolina State University, USA)
Co-organiser: Anthony Bloch (University of Michigan, Ann Arbor, USA)

This minisymposium focuses on a wide range of applications of geometric methods to dynamics, mechanics, and control. The following areas will be addressed, among others: dynamics and bifurcations in networks of identical coupled systems, exponential maps, reduction theory, decoding algorithms from the dynamical system point of view, and a dynamical system approach to control and stabilization. The unifying theme is the use of geometrical methods in dynamical systems.

A connection theoretic approach to reduction of second-order dynamical systems with symmetry. **Tom Mestdag** (The University of Michigan, USA) IC/MT1434/034

There are several different geometric contexts in which we find manifestations of the following behaviour: roughly speaking, there is a system of second-order ordinary differential equations which admits a Lie group of symmetries; this system is reduced to a coupled pair of sets of equations, one of second-order (albeit in a generalized sense) and one of first-order. Some examples are: the geodesics of a manifold with a Kaluza-Klein metric (Wong's equations); simple mechanical systems with symmetry, including control systems; Lagrangian reduction (Lagrange-Poincare equations) and non-abelian Routh reduction (Lagrange-Routh equations). In different cases different auxiliary geometrical structures are required to carry out the reduction. In the present talk we shall explain the nature of this reduction process for a dynamical system governed by second-order differential equations, which is invariant under a Lie group action, using thus the simplest type of auxiliary machinery imaginable. We show that, in fact, the systems decompose in three parts. It is our aim to explain how this decomposition arises, with the help of connection theory; and to discuss the processes of reduction and reconstruction from this standpoint.

Discrete mechanics and control on Lie groupoids. **Eduardo Martínez** (Universidad de Zaragoza, Spain) IC/MT1990/034

Discrete Lagrangian Mechanics on Lie groupoids was introduced in[1] and further developed in[2]. This formalism allows to describe the discrete analogs of continuous systems on Lie algebroids, as can be obtained, for instance, by an adequate discretization.

Such results can be naturally extended for discrete-time optimal control problems defined on Lie groupoids. By an adequate study of the admissible variations we will find the optimality conditions, that will be expresed in terms of composability in a groupoid.

We will show some examples and we will further study symmetry and reduction theory. In particular, the discrete Euler-Lagrange equations for a discrete mechanical system on a Lie groupoid are obtained as a particular case.

[1] A. Weinstein; Lagrangian Mechanics and groupoids. Fields Inst. Comm. **7** (1996) pp.207–231.

[2] Marrero, J.C., Martín de Diego, D. and Martínez, E.; Discrete Lagrangian and Hamiltonian mechanics on Lie groupoids, Nonlinearity **19** (2006) pp.1313–1348.

Systems theoretic questions in coding theory. **Joachim Rosenthal** (Universität Zürich, Switzerland) IC/MT1790/034

A central theme of current research in coding theory are low density parity check (LDPC) codes and more general codes defined via graphs. There exist various decoding algorithms which work in a decentralized manner and which can be viewed as a discrete dynamical system. In this talk we explain these algorithms from a systems theoretic point of view.

Stabilization of discrete mechanical systems. **Dmitry Zenkov** (North Carolina State University, USA), Anthony Bloch (University of Michigan, Ann Arbor, USA), Melvin Leok (Purdue University, USA), Jerrold Marsden (California Institute of Technology, USA) IC/MT1124/034

In this talk we discuss the controlled Lagrangian approach to feedback stabilization of discrete mechanical systems with symmetry. We describe new phenomena that arise in the controlled Lagrangian approach for mechanical systems in the discrete context. We also discuss digital and model predictive controllers.

IC/MP279/034: Geometry, dynamics, and control. #2

Organiser: Dmitry Zenkov (North Carolina State University, USA)
Co-organiser: Anthony Bloch (University of Michigan, Ann Arbor, USA)

(For abstract, see session #1 above.)

Bifurcations in small networks of identical coupled systems. **Martin Golubitsky** (University of Houston, USA) IC/MT1784/034

There are many special features that occur generically in bifurcations from synchrony in small networks of differential equations. The situation is reminiscent of bifurcations in systems with symmetry, but here the special mathematical structure is due to the way that the identical systems are coupled. We discuss several surprising examples of generic bifurcations that occur in small networks.

Convexity, reduction, and dynamics. **Tudor Ratiu** (École Polytechnique Fédérale de Lausanne, Switzerland) IC/MT2754/034

Convexity properties of momentum maps are intimately related to bifurcation phenomena in Hamiltonian systems with symmetry. This talk surveys recent progress in the convexity properties induced by symplectic actions and their relationship to reduction theory. The most general convexity theorem is associated to an arbitrary symplectic action of a Lie group, is metric in nature, and does not require the existence of a momentum map. The results presented in this survey are based on several papers written jointly with P. Birtea and J.-P. Ortega.

Geometry of integrable systems and optimal control. **Anthony Bloch** (University of Michigan, Ann Arbor, USA) IC/MT2361/034

In this talk I will discuss the dynamics and geometry of certain dynamical systems arising from optimal-control problems and the maximum principle . In particular I will discuss various integrable Hamiltonian systems that arise in this context. This includes the study of various geodesic flows on manifolds including Stiefel manifolds, the study of generalized rigid body equations and certain subRiemannian optimal control problems. I will discuss such systems in both the smooth and discrete settings.

Riemannian exponential maps of the diffeomorphism group on a flat 2D-torus. **Thomas Kappeler** (Universität Zürich, Switzerland), Enrique Loubet (ETH Zürich, Switzerland), Peter Topalov (Northeastern University, USA) IC/MT1877/034

We study exponential maps induced by Sobolev type right-invariant weak Riemannian metrics of order $k \geq 0$ on the Lie group of smooth, orientation preserving diffeomorphisms of the two dimensional torus and prove that for $k \geq 1$, but not for $k = 0$, each of them defines a smooth Frechet chart of the identity.

IC/MP40/036: Euler and space exploration.

Organiser: Martin Lo (Jet Propulsion Laboratory, USA)

The exploration of space is typically thought of as an engineering endeavor, but actually, mathematics, both pure and appliced, play a very important role. Euler is a case in point: his work on the Three Body Problem is today one of the cornerstones of modern astrodynamics. This minisymposium will describe some of the latest research and development on space missions, like the James Webb Telescope, where Euler's work plays a key role.

Central to this is dynamical systems theory, first studies in Poincare's seminal work on the Three Body Problem where he discovered dynamical chaos. Today, chaotic orbits enable numerous ultra-low-fuel missions around the Solar System. Recent work has shown that the transport of materials in the Solar System is governed by the chaotic dynamics of the collinear solutions that Euler discovered some three centuries ago, what we now call the L1, L2, and L3 *Lagrange Points*. Several of our speakers first introduced this approach to space mission design and will describe their latest work on the subject.

Although the dynamics of Euler's solutions play a fundamental role in the design of these trajectories, the use of advanced propulsion technology created many new and challenging problems. In particular the optimization of trajectories using low thrust ion engines is highly complex and interesting. Several of our speakers will address this problem.

Another interesting problem is the use of of satellites flying in formation around L2. They are typically used for astronomy missions that require long baseline interferrometers. Some of our speakers will describe the precision control of these formations in this highly nonlinear regime.

Euler would be delighted and amazed to find how his collinear orbits have made such a huge impact on space exploration and our understanding of the chaotic dynamics of the Solar System.

Space-craft insertion in unstable environments: application to formation flight near the libration points. **Benjamin Villac** (UC Irvine, USA) IC/MT4493/036

The stable manifold associated with the periodic and quasi-periodic orbits has proved a key concept for the low cost transfer of spacecraft to libration point regions. Recent interest in formation flight near the libration points opens the question of precise spacecraft insertion along a nominal orbit. While current approaches emphasize the station-keeping and (re)configuration of such formation – and thus consider the insertion problem from a control viewpoint –, we propose a purely dynamical mechanism for spacecraft insertion and servicing in formation flight. By analyzing the rate of convergence of the orbits on the stable manifolds of the target libration point trajectory, opportunities for low cost transfer to a specific location on the target orbit are determined.

Invariant manifolds and the interplanetary super-highway. **Martin Lo** (Jet Propulsion Laboratory, USA) IC/MT4494/036

The classical view of the Solar System since the time of Copernicus and Kepler is an orderly universe centered on the Sun with the planets revolving in isolated near-circular orbits. But the work of Wisdom and Laskar have shown the Solar System is not so regular and orderly, but instead, it is chaotic. At the heart of this chaos are the invariant manifolds associated with the 3-body solutions discovered by Euler, what is now called the collinear Lagrange Points. If we view the Solar System as a series of coupled 3-body problems, these manifolds intersect in configuration space and sometimes in phase space to provide an ultra low energy transport from the Kuiper Belt to the Sun. This is the *Interplnaetary Superhighway* which plays a significant role in the transport and morphology of the Solar System from the zodiacal dust, the rings, the asteroid belt, to the comets.

In the 1960s Farquhar discovered the 3-dimensional periodic *halo orbits* around the collinear Euler points. In 1978, the first space mission flew in this unique orbit under Farquhar's leadership. During the 1980s the Barcelona school under Carles Simo, Gerard Gomez, and their colleagues, introduced the use of dynamical systems theory to the design of space trajectories. This work inspired Howell and Lo to apply invariant manifolds to NASA missions in the mid 1990s. This led to the design of the Genesis trajectory by Lo and Howell's group using the heteroclinic behavior between L1 and L2. It also inspired the investigation that led to Lo's discovery of the Interplanetary Superhighway with the help of his student Ross. In order to understand the heteroclinic dynamics of the Genesis orbit, Lo turned to Marsden and his student Koon for help. Together, they extended the work of Llibre, Martinez and Simo on homoclinic orbits to heteroclinic orbits to explain the Genesis orbit.

We will discuss the implications of this network in our Solar System for science and space exploration.

Leaving and reaching the moon from a libration-point orbit. **Gómez-Muntané Gerard** (Universitat de Barcelona, Spain), Masdemont Josep (Universitat Politècnica de Catalunya, Spain), Elisa Maria Alessi (Universitat de Barcelona, Spain) IC/MT4499/036

Using the hyperbolic invariant manifolds of the central manifolds of L1 and L2 in the Earth–Moon system, we explore the collision orbits with the surface of the Moon. Applications to mission analysis and astronomy will be presented.

Low-thrust mission analysis methods and results for the ESMO-SEP mission. **Daniel Novak** (University of Glasgow, UK), Jeannette Heiligers (TU Delft, The Netherlands), Camilla Colombo (University of Glasgow, UK), Massimiliano Vasile (University of Glasgow, UK) IC/MT4997/036

The European Student Moon Orbiter (ESMO) mission aims at injecting a micro-satellite class spacecraft into an orbit around the Moon by 2011. In addition to the scientific goal, the whole project aims at a design completely carried out by several students over Europe, working together in a virtual concurrent engineering environment. The stringent requirements on the cost and the reliability of the mission have a strong impact on the mission analysis: the trajectory must be reliable (to minimise the risks), the transfer time should be as short as possible, and ground stations must be chosen accurately (to reduce the ground segment cost). This paper focuses on one of the two investigated options for the transfer to the Moon: a low-

thrust transfer through the Lagrangian point L_1. The transfer trajectory is composed of a spiral winding up from a GTO to almost L_1, transfer through the neighbouring region of L_1 and final spiral winding down to an orbit that can guarantee six months of operations. The paper will present the complete mission analysis for the low-thrust option in addition to a description of the methodology used to design the low-thrust, low-energy transfer through L_1.

IC/MP40/036: Euler and space exploration. #2

Organiser: Martin Lo (Jet Propulsion Laboratory, USA)

(For abstract, see session #1 above.)

BepiColombo gravitational capture and the elliptic restricted three-body problem. **Stefano Campagnola** (University of Southern California, USA), Martin Lo (Jet Propulsion Laboratory, USA) IC/MT4544/036

BepiColombo is the cornerstone ESA-approved mission to Mercury. It will reach its destination in 2019, after a nearly 5-year long transfer using multiple gravity assists and low-thrust propulsion. To avoid a single point failure of a classical chemical orbit insertion burn, an arrival scenario was implemented where the gravity of the Sun is exploited to weakly capture the spacecraft in a Mercury orbit. This technique can be better understood in the frame of the elliptic three-body problem model. In particular, Gravitational Capture conditions are investigated, together with the allowed region of motions for the spacecraft.

Challenges of NASA prospective libration missions. **David Folta** (NASA Goddard Space Flight Center, USA) IC/MT4548/036

As the future unfolds for NASA in its pursuit of the Vision for Space Exploration, libration orbits play a prominent role. Both Sun-Earth and Earth-Moon regions will be exploited requiring mathematical advancements and comprehensive demonstrations. With several successful single missions, new challenges of formation flying, intra-transfer orbits, and unique station-keeping strategies take center stage. Mathematical applications to improve and otherwise optimize mission parameters are necessary to permit communication and exploration architectures of the exploration vision. Recent advancements, which apply EulerŠs grid technique, is one example. The paper focuses on potential missions and how recent advancements based on EulerŠs imaginings make these missions possible.

Design strategies for libration-point missions: theory to application. **Kathleen Howell** (Purdue University, USA) IC/MT4549/036

Spacecraft missions to the libration points in sun–planet and planet–moon systems are of increasing interest. A number of such missions have already been launched. As the theoretical understanding of the dynamical structure in these regions of space expands, however, trajectory design to support actual mission requirements is more complex. Baseline trajectories for some recent mission scenarios are presented. Example approaches for transition of the designs to higher fidelity models is discussed.

IC/MP344/036: Mathematical models and computational methods for nano- and bio-technologies.

Organiser: Roderick Melnik (Wilfred Laurier University, Canada)
Co-organiser: Jack Tuszynski (Cross Cancer Institute, Edmonton, Canada)

Most cutting edge developments that are taking place in nano and bio-technologies rely heavily on advances in mathematical modeling and computational methodologies. Examples include, but not limited to, new technologies based on low-dimensional semiconductor nanostructures such as quantum dots, nanotubes, sensors and actuators, drug discovery methodologies, protein- and macrotubule-based devices, techniques, and processes in designing biomolecular motors.

Development and integration of mathematical modeling techniques into these nano- and bio- technologies is an essential pre-requisite for further progress in this increasingly inter-disciplinary field. At the same time, problems that are arising from the development of new nano- and bio- technologies present challenges to applied mathematicians, stimulating advances in differential, difference, and integral equations, numerical analysis and computational mathematics among other fields.

This minisymposium has two aims. The first is to demonstrate some of the key mathematical and computational challenges associated with the state-of-the-art developments in new nano- and bio-technologies, focusing on several representative examples. The second is to expose the more technologically oriented part of the community to most advanced mathematical and computational techniques that are currently being developed in the field, and thus to encourage inter-disciplinary collaborations.

On the interconvesion integral equation for relaxation and creep. **Robert Anderssen** (CSIRO, Australia), Frank de Hoog (CSIRO, Australia) IC/MT1401/036

Because of the particularization of genetic activity that they perform, rheological phenotypes are playing an increasingly important role in biotechnology research including quantitative trait loci (QTL) analysis. For the determination of such phenotypes, the viscoelastic nature of biomaterials must be taken into account. The rheological characteristics of viscoelasticity are normally modelled, as a function of the time t, in terms of the relaxation $G(t)$ and the creep (retardation) $J(t)$ functions. Different instruments are available for performing the associated relaxation and creep experiments, which generate the stress-strain relaxation and creep data from which estimates $G_{est}(t)$ and $J_{est}(t)$ of $G(t)$ and $J(t)$ are recovered. In many situations, only a single instrument is available which can only perform on of these experiments. Consequently, there is considerable interest in computational techniques which allow $J_{est}(t)$ or $G_{est}(t)$ to be determined from the other using the interconversion relationships

$$\int_{)}^{t} G(t-s)J(s)ds = \int_{0}^{t} J(t-s)G(s)ds = t.$$

Though this matter has been examined numerically in the rheological literature, a formal mathematical comparison of the two possibilities has never been undertaken. This talk will report on the results from recent mathematical investigations.

Coupled nonlinear effects in nano-structures and their applications. **Roderick Melnik** (Wilfred Laurier University, Canada) IC/MT3238/036

We demonstrate that the conventional application of linear mathematical models to the analysis of optoelectronic properties of nanostructures in bandstructure engineering may be inadequate for new emerging applications. Examples are given for several types of low-dimensional semiconductor nanostructures, where we account consistently for nonlinear strain and piezoelectric effects in calculating their properties, and for carbon nanotube based devices such as field emitting diodes. A major focus in this talk is given to the analysis of quantum dots, where it is essential to account for coupled effects.

This is a joint work with R. Mahapatra, N. Sinha, J.T.W. Yeow, D.A. Jaffray, M. Willatzen, B. Lassen, and L. Lew Yan Voon

Computational models for the numerical simulation of voltage-operated channels in nano-bio-electronics. **Riccardo Sacco** (Politecnico di Milano, Italy), Bice Chini (Consiglio Nazionale delle Ricerche, Italy), Joseph Jerome (Northwestern University, USA), Massimo Longaretti (Politecnico di Milano, Italy), Giovambattista Marino (Politecnico di Milano, Italy) IC/MT1388/036

In this lecture, a novel mathematical and computational model is proposed for the numerical simulation of Voltage Operated ionic Channels (VOC) in Nano–Bio–Electronics applications. This is a first step towards a multi–physics description of hybrid bio–electronical devices such as bio–chips. The model consists of a coupled system of nonlinear partial differential equations, comprising a Poisson-Nernst-Planck system to account for electro-chemical phenomena, and a Navier–Stokes system to account for fluid–mechanical phenomena. Suitable functional iteration techniques for problem decoupling and finite element methods for discretization are proposed and discussed. Numerical results on realistic VOCs illustrate the validity of the model and its accuracy by comparison with relevant computed channel equivalent electrical parameters with measured data.

Can we predict DNA biological activity by modelling its fluctuations?. **Michel Peyrard** (École Normale Supérieure de Lyon, France), Santiago Cuesta Lopez (École Normale Supérieure de Lyon, France), Dimitar Angelov (École Normale Supérieure de Lyon, France), Titus Van Erp (Katholieke Universiteit Leuven, Belgium), Johannes-Geert Hagmann (École Normale Supérieure de Lyon, France) IC/MT1563/036

DNA dynamics is essential for its biological function. The genetic code could not be read without a local unwinding of the double helix, and large openings, the so-called "DNA bubbles", are supposed to allow the formation of some specific DNA structures such as the T-loop that stabilises the end of the chromosomes, or to affect the binding of proteins.

Mesoscopic models give a fairly accurate description of the thermal denaturation of DNA, i.e. the separation of the two strands by heating, and they predict the existence of localised fluctuations which are reminiscent of the "breathing" of the double helix observed by biologists. Thus it is tempting to try to use these models to predict the biological activity of DNA.

From experimental studies it has been speculated that the formation of bubbles of several base-pairs length, due to thermal fluctuations, is an indication of biologically active sites. A comparison between molecular dynamics simulations of the PBD model of DNA and experiments suggested that calculations could be used to detect such sites [1], but this observation is however not very reliable because the occurrence of large bubbles is rare, even in long simulations, so that the statistical significance of the results can be questioned.

We introduce a method that is orders-of-magnitude faster than molecular dynamics to analyse these bubbles [2,3] and discuss experiments which measure the local fluctuations of DNA as a function of its sequence. We show how they can be used to improve present models to make them more accurate to describe DNA properties [4], and ultimately approach the goal of determining the fluctuations of heterogeneous DNA sequences from physical studies of a highly simplified model and understanding their relation to biological activity.

[1] Chu H. Choi, G. Kalosakas, K. O. Rasmussen, M. Hiromura, A.R. Bishop and A. Usheva, *DNA dynamically directs its own transcription initiation* Nucleic Acid Research **32** 1584-1590 (2004)

[2] Titus S. van Erp, Santiago Cuesta-Lopez, Johannes-Geert Hagmann, Michel Peyrard, *Can one predict DNA Transcription Start Sites by studying bubbles?* Phys. Rev. Lett. **95**, 218104 (2005)

[3] Titus S. van Erp, Santiago Cuesta-Lopez, and Michel Peyrard, *Bubbles and the denaturation in DNA.* Eur. Phys. J. E **20**, 421-434 (2006)

[4] Santiago Cuesta-Lopez, Dimitar Angelov and Michel Peyrard, unpublished.

IC/MP344/036: Mathematical models and computational methods for nano- and bio-technologies. #2

Organiser: Roderick Melnik (Wilfred Laurier University, Canada)
Co-organiser: Jack Tuszynski (Cross Cancer Institute, Edmonton, Canada)

(For abstract, see session #1 above.)

Multiscale simulations of complex materials for engineering and biological applications. **Simone Melchionna** (Università degli Studi di Roma "La Sapienza", Italy), Efthimios Kaxiras (Harvard University, USA) IC/MT2355/036

A variety of physical phenomena involve multiple length and time scales. In such systems, the changes in bonding and atomic configurations at the microscopic, atomic level have profound effects on the macroscopic properties, be they of mechanical or electrical nature. Linking the processes at the two extremes of the length scale spectrum is the only means of achieving a deeper understanding of these phenomena and, ultimately, of being able to predict and control them.

While methodologies for a single scale are well developed in many fields of physics, chemistry or engineering, methodologies that couple scales present important challenges at the conceptual and computational level. In this talk we review the development of methodologies for simulations across disparate length scales and present illustrative examples, including hydrogen embrittlement of metals [1], DNA conductivity and translocation through nanopores [2], and the use of surface chemical modification to control the wettability of surfaces for biological applications [3].

[1] ŞFrom electrons to finite elements: a concurrent multiscale approach for metalsŠŠ G. Lu, E. Tadmor and E. Kaxiras, Phys. Rev. B 73, 024108 (2006).

[2] ŞCarbon nanotube interaction with DNAŤ, G. Lu, P. Maragakis and E.Kaxiras, NanoLett. 5, 897-900 (2005).

[3] ŞTuning solid surfaces from hydrophobic to superhydrophilic by submonolayer surface modificationŤ, S. Meng, Z.Y. Zhang and E. Kaxiras, Phys. Rev. Lett. 97, 036107 (2006).

The role of nonlinearities in the biophysical properties of cytoskeletal components. **Jack Tuszynski** (Cross Cancer Institute, Edmonton, Canada) IC/MT2982/036

This paper discusses the role of nonlinearities in the physical description of several key biomolecules that participate in a number of crucial subcellular processes, namely actin, microtubules and ions crowding around these filaments. We show that the assembly kinetics of actin is a nonlinear process that requires not only a mechanism of saturation but also annealing and fragmentation that are governed by coupled nonlinear equations involving monomer concentration and filament number as the key dynamical variables. The observed dendritic growth of actin networks in cell motility phenomena is subsequently described by the coupling of actin filaments to the protein called Arp 2/3. We then investigate the role of nonlinear dynamics in the formation of microtubules. First of all, spaceflight laboratory experiments have shown that the in vitro and in vivo self-organization of microtubules is sensitive to gravitational conditions. We propose a model of self-organization of microtubules in a gravitational field. The model is based on the dominant chemical kinetics. The pattern formation of microtubule concentration is obtained: 1) in terms of a moving kink in the limit when the disassembly rate is negligible, and 2) for the case of no free tubulin and only assembled microtubules present. The results of our simulations are in good quantitative agreement with experimental data. Next, we present a recently proposed model of molecular and bulk elastic properties of microtubules that include macroscopic estimates of the anisotropic elastic moduli of microtubules, accounting for the molecular forces between tubulin dimers: for a longitudinal compression, for a lateral force and for a shearing force. At the level of large bending motions of microtubule filaments, a continuous medium model is proposed describing a microtubule as an elastic rod. Keeping the dominant nonlinear terms in the bending dynamics equation, we found that when the microtubule is subjected to bending forces, the deviation angle satisfies a Sine-Gordon equation. Particular analytical solutions of this equation are found which describe kink and anti-kink bending modes that may propagate at a range of velocities along the length of the microtubule. Kinetic energies and characteristic damping times of these modes are calculated for different propagation velocities and compared with thermal and ATP hydrolysis energies. Finally, we discuss how coupled differential equations describing the interactions between ions in solution and the filament they surround can lead to solitonic signal transmission.

The walking molecules kinesin *and* myosin. **Hannes Bolterauer** (Universität Gießen, Germany) IC/MT3739/036

We discuss the principal ideas of existing models for kinesin, NCD and Myosin, which are existing motorproteins inside the cell. We find that in order to explain uni-directionality, but also the different directions of walking of ordinary Kinesin and NCD, we cannot use one-dimensional models or quasi-one-dimensional models. Instead we have to describe the two heads as extended objects in an, at least, two-dimensional space. Our model of directed binding uses the natural elasticity of the molecules and explains the general excepted hand over hand movement in different directions. We establish the Langevin and Fokker–Planck description and try to solve it. Our results are in agreement with existing experiments. The described mechanism could be a basis to construct artificial molecular motors.

03: Nonlinear Analysis and Dynamical Systems, Contributed Talks

IC/CTS4660/03: **Stochastic modelling.**

Organiser: Vasile Berinde (North University of Baia mare, Romania)

Modeling the asynchronous circuits: absolutely inertial delays. **Serban Vlad** (Oradea City Hall, Romania) IC/CT702/015

The detail level modeling of the asynchronous circuits from the digital electrical engineering (logical gates and wires) is made with the mathematical models of the delay circuits, called delays and with Boolean functions. A delay is a multi-valued function f that associates to each input $u : \mathbf{R} \to \{0,1\}$ a set of states $x \in f(u), x : \mathbf{R} \to \{0,1\}$ so that a stability property be fulfilled. We suppose the existence of $\delta_r \geq 0, \delta_f \geq 0$ so that for all u and all $x \in f(u)$ the switch of x from 0 to 1 (from 1 to 0) implies that x remains constant equal with 1 (constant equal with 0) more than δ_r time units (than δ_f time units); then f is called absolutely inertial.

The work analyses the absolutely inertial delays from the point of view of the order, the duality, the serial connection, the intersection, the union and the time invariance. Alternative definitions of absolute inertia and several examples are given. We eventually define a special case of absolutely inertial delays, the Zeno delays.

Empirical study of the rate of convergence of some fixed point iterative methods. **Vasile Berinde** (North University of Baia mare, Romania), Mădălina Păcurar (Universitatea Babeş-Bolyai, Romania) IC/CT1859/003

From a practical point of view (that is, from a *numerical* point of view), a fixed point theorem is valuable if, apart of ensuring the existence (and possible, uniqueness) of the fixed point, it satisfies at least the next two requirements (see, e.g., [1]):

(a) it is able to provide an error estimate for the iterative process used to approximate the fixed point;
(b) it provides explicit information on the stability of this iterative method or, equivalently, on the data dependence of the fixed point.

Only a few fixed point theorems in literature are known to fulfill the two requirements and, generally, this is done mainly for the Picard iteration in conjunction with various strong contractive type conditions. Under weaker contractive conditions, the general problem of studying the rate of convergence of fixed point iterative methods arises usually into the next two different contexts, see [2,3,4,5]:

1) For a certain fixed point iterative method (Picard, Krasnoselskij, Mann, Ishikawa etc.) we do not know an *analytical* error estimate. In this case we can try an *empirical* study of the rate of convergence.
2) For large classes of operators (like quasi-contractions) two or more fixed point iteration procedures are known to be able to approximate the fixed points. In such situations, it is of theoretical and practical importance to compare these methods with regard to their convergence rate, in order to establish, if possible, which one converges faster, w.r.t. a certain concept of rate of convergence.

The main aim of this paper is to illustrate how, in the absence of theoretical results, we can perform an empirical study of the rate of convergence of fixed point iterative methods, using the FIXPOINT software package, specially designed for this purpose. The empirical approach of the rate of convergence of fixed point iteration procedures was firstly considered by B.E. Rhoades [6,7,8]. This problem is still of real scientific interest and perspective because it also offers the possibility of inferring theoretical rate of convergence from empirical observations, like in [2,3], which could be very useful when applying these methods to solve concrete problems of industrial and applied mathematics. A survey of the most significant results in this area, together with some open problems, are finally pre-

sented.

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An evaluation of test statistics for detecting temporary change in $BL(1,1,1,1)$ models. **Azami Zaharim** (Univeristi Kebangsaan, Malaysia), Amiruddin Ismail (Subang Jaya, Malaysia), Shahrum Abdullah (Universiti Kebangsaan Malaysia), Ibrahim bin Mohamed (University of Malaya, Malaysia), Ibrahim Ahmad (Univeristi Kebangsaan, Malaysia) IC/CT4462/032

A study is carried out to investigate the sampling properties of the outlier test statistics of a procedure developed for detecting temporary change in $BL(1,1,1,1)$ processes. It is done with respect to the sample size, the type of outlier and the size of the coefficients of the $BL(1,1,1,1)$ process. The results show that, in general, the outlier detection procedure is capable of detecting TC, although the performance is affected if is large.

On a stochastic robust control. **Mamoud El-Borai** (Alexandria University, Egypt) IC/CT46/034

We consider some stochastic dynamical systems,which represents robustness that arise in controller and filter designs and also represent a remote control system in the presence of a network cable. The flexible arms connected by elastic joints of the robot is also studied. In addition we introduce a theory about the artificial intelligence. Some deterministic fractional dynamical systems is studied. These systems have many applications in robot and industry.

Keywords: Stochastic dynamical systems,stochastic robust control,flexible arms, artificial intelligence.

Nonlinearity management in optics. **Mason Porter** (Oxford Univ. UK & Caltech, USA) IC/CT4366/033

We present experimental, computational, and theoretical results concerning pulse stabilization and modulational instabilities in nonlinear optics by implementing "nonlinearity management" using layered Kerr media. The theoretical framework describing this system is a nonlinear Schrödinger (NLS) equation with a piecewise constant nonlinearity coefficient.

IC/CTS4671/03: Modeling and analysis of physical systems.

Organiser: Shu-Ming Chang (National Tsing Hua University, Taiwan)

Asymptotics for some vibro-impact problems with a linear dissipation term. **Laetitia Paoli** (Université Saint-Etienne, France), Alexandre Cabot (Université de Limoges, France) IC/CT3926/033

Given $\gamma \geq 0$, let us consider the following differential inclusion

$$(S) \qquad \ddot{x}(t) + \gamma \dot{x}(t) + \partial\Phi(x(t)) \ni 0, \qquad t \in \mathbb{R}_+,$$

where $\Phi : \mathbb{R}^d \to \mathbb{R} \cup \{+\infty\}$ is a lower semicontinuous convex function such that int(dom Φ) $\neq \emptyset$. The operator $\partial\Phi$ denotes the subdifferential of Φ. When $\Phi = f + \delta_K$ with $f : \mathbb{R}^d \to \mathbb{R}$ a smooth convex function and $K \subset \mathbb{R}^d$ a closed convex set, inclusion (S) describes the motion of a discrete mechanical system subjected to the perfect unilateral constraint $x(t) \in K$ and submitted to the conservative force $-\nabla f(x)$ and the viscous friction force $-\gamma \dot{x}$. We define the notion of *dissipative* solution to (S) and we prove the existence of such solutions with conservation (resp. loss) of energy at impacts. If $\gamma > 0$ and $\Phi_{|\mathrm{dom}\Phi}$ is locally Lipschitz continuous, any dissipative solution to (S) converges, as $t \to +\infty$, to a minimum point of Φ. When Φ is strongly convex, the speed of convergence is exponential. Assuming as above that $\Phi = f + \delta_K$, suppose that the boundary of K is smooth enough and that the normal component of the velocity is reversed and multiplied by a restitution coefficient $r \in [0,1]$ while the tangential component is conserved whenever $x(t) \in \mathrm{bd}(K)$. We prove that any dissipative solution to (S) satisfying the previous impact law with $r < 1$ is contained in the boundary of K after a finite time. The case $r = 1$ is also addressed and leads to a qualitatively different behavior.

Dynamics in Bose–Einstein condensates. **Shu-Ming Chang** (National Tsing Hua University, Taiwan) IC/CT1385/033

We derive the asymptotic motion equations of vortices for the time-dependent Gross-Pitaevskii equation with a harmonic trap potential. The asymptotic motion equations form a system of ordinary differential equations which can be regarded as a perturbation of the standard Kirchhoff problem. From the numerical simulation on the asymptotic motion equations, we observe that the bounded and collisionless trajectories of three vortices form chaotic, quasi 2- or quasi 3-periodic orbits. Furthermore, a new phenomenon of $1:1$-topological synchronization is observed in the chaotic trajectories of two vortices. On the other hand, we study the distribution of m segregated nodal domains of the m-mixture of Bose-Einstein condensates under positive and large repulsive scattering lengths. It is shown that components of positive bound states may repel each other and form segregated nodal domains as the repulsive scattering lengths go to infinity. Efficient numerical schemes are created to confirm our theoretical results and discover a new phenomenon called verticillate multiplying, that is, the generation of multiple verticillate structures. In addition, our proposed Gauss-Seidel-type iteration method is very effective in that it converges linearly in 10 to 20 steps.

Mathematical modeling of rhythmic and pulsatile GnRH hormone secretion by synchronized GnRH neurons based on a robust mechanism. **Anmar Khadra** (University of British Columbia, Canada), Yuexian Li (University of British Colombia, Canada) IC/CT4352/036

Gonadotropin Releasing hormone (GnRH) secreted by GnRH neurons plays an essential role in the onset and progression of reproductive maturation, and regulation of hormonal changes that occur during menstrual and estrous cycle. There is a strong evidence suggesting that these GnRH neurons are capable of generating pulsatile and episodic neurosecretion of this hormone intrinsically. However, the underlying mechanism for the GnRH-pulse generator remains largely unknown. The presence of GnRH receptors on these neurons allow GnRH hormone to exert autocrine regulation on its own release. This led a group of experimentalist at NIH to propose in 2003 a mechanism describing this effect. We later developed in 2006 a mathematical model based on this proposed mechanism. The model was further extended to study synchrony in GnRH neurons by incorporating the idea of a common pool of GnRH hormone.

We shall present in this talk the mathematical model and few important aspects of it. We shall show that a heterogeneous family of coupled GnRH neurons is capable of secreting the hormone synchronously. In fact, we show that only 50neurons need to be active for pulse generation. The effects of averaging in the parameter-values, as well as the volume of the extracellular medium will be also discussed. In addition, several model predictions explaining the type of behaviour observed experimentally upon the injection of GnRH-agonist will be stated. These results will demonstrate the robustness of this process.

Weight-function for a crack in an orthotropic medium under impact-shear loading. **Subir Das** (B.P. Poddar Institute, India) IC/CT4176/009

The paper deals with the investigation of elastodynamic response of an infinite orthotropic medium containing a central crack under impact shear loading. Laplace and Fourier integral transforms are employed to reduce the dimensional wave propagation problem to the solution of a pair of dual integral equations in the Laplace transformed plane. These integral equations are then reduced to integral differential equations which have been solved in the low frequency domain by method of iteration. To determine time dependence, these equations are inverted to yield the dynamic stress intensity factor (SIF) for shear point force loading. These results have been used to obtain the SIF at the crack tip which corresponds to the weight function for the crack under shear loading. Analytical expressions of the weight function is used to derive SIF for polynomial loading.

Interfacial Griffith cracks between bonded dissimilar media. **Sudipta Chakraborty** (B.P.Poddar Institute, India) IC/CT4580/094

The paper deals with the interaction of a pair of outer cracks on a central crack situated at the interface of two dissimilar orthotropic half planes. The mixed boundary value problem is reduced to solving a pair of simultaneous singular integral equations which have finally been solved numerically by using Jacobi polynomials. The analytical expressions for stress intensity factors at the central crack tip and the expression of the strain energy release rate have been derived for general loading. Numerical values of the interaction effects of the outer cracks on the central crack have been calculated through stress magnification factors. It is seen that the interaction effects are either shielding or amplification depending on the size of the outer cracks and their spacing from the central crack.

IC/CTS4667/03: Numerical methods for nonlinear ODEs.

Organiser: Changpin Li (Shanghai University, PR China)

Nonlinear time-series modelling and prediction using correlation analysis. **Andrzej Dydynski** (Politechnika Warszawska, Poland), Jarosław Arabas (Politechnika Warszawska, Poland) IC/CT3038/032

We present a novel way for time series prediction. The method is based on the correlation analysis and allows for handling nonlinearities of different type and character. The presented approach results in an approximation model that combines nonlinear units taken from radial basis functions (RBF) and from multilayer perceptrons (MLP). The approach leads to a low mean error of the approximation with a number of parameters significantly smaller when compared to RBF and MLP.

The main problem in the system identification is to find a good model structure. Many widely used nonlinear approximators (e.g., MLP or RBF) are linear combinations of nonlinear functions, called *base functions*. A larger model which contains more parameters is more likely to adapt to any nonlinear function but at the same time it is more likely to overfit. Here we present an Incrementally Built Heterogenous Model (IBHM) for modeling nonlinear systems by regression. The approach combines elements of several models in a single model structure.

The model is a weighted sum of base function and is incrementally expanded by adding one of many possible candidate base functions. The candidate base functions are inspired by artificial neurons from MLP and RBF. In each iteration of the IBHM method, a residue function being the difference between the approximated function values and the model output is computed. Then each candidate base function is scored according to the degree in which it resembles the residue function; a correlation measure is used for that purpose. The highest score candidate is included as a base function to the model, and the weight values assigned to base functions are recomputed. The process is repeated until a certain stop criterion is attained.

The idea of incremental model building has been raised by several authors, but usually it was constrained to homogenous models only, that is to models which used similar functional form of base functions. Probably the best known methods are Group Method of Data Handling (GMDH, originally used for polynomial models and then for MLP) [9] and Cascade Correlation method for MLP [8]. Moreover, in contrary to our approach, where the base function is selected basing on the residue function only, the aforementioned methods usually expand the model by a base function and then tune its parameters and weights.

In this paper we introduce the IBHM method and illustrate its properties using the benchmark data for time series prediction.

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Two-state model of excitable system with time delayed feedback: renewal theory approach. **Andrey Pototsky** (Loughborough University, UK), Natalia Janson (Loughborough University, UK) IC/CT4562/031

We present a two-state model of an excitable system with time delayed feedback control. The two-state stochastic process can be interpreted as a renewal process with history-dependent residence time distributions (RTDs). The equilibrium RTDs in the sense of the averaging over all possible histories are introduced. Assuming that the transition rates are known functions of the history we derive an equation for the equilibrium RTDs for arbitrary delay time. We analytically solve this equation for moderate delay times in the case when the duration of the excited state is not affected by the noise. Analytic results are compared with numerical simulations of a bistable system with two time delays. Using the combination of the renewal theory power spectrum and the derived analytic expression for the equilibrium RTD, the piece-wise linear dependence of the main period of the noise-induced oscillations on the delay time is demonstrated. Delay-induced onset and enhancement of the coherence resonance is shown for positive feedback strength.

Stability analysis for nonlinear fractional differential systems. **Changpin Li** (Shanghai University, PR China) IC/CT467/038

In 1695, Leibniz wrote a letter to L'Hôpital and discussed whether or not the meaning of derivatives with integer orders could be generalized to derivatives with non-integer orders. L'Hôpital was somewhat curious about the problem and asked a simple question in reply: ŞWhat if the order will be 1/2?Ť. Leibniz in a re-reply letter dated September 30 of the same year, anticipated: ŞIt will lead to a paradox, from which one day useful consequences will be drawn.Ť The date September 30, 1695, is regarded as the exact birthday of the fractional calculus. In the following centuries, the theories of fractional calculus (fractional derivatives and integrals) underwent a significant and even heated development, primarily contributed by pure, not applied, mathematicians. The question put forward by Leibniz for a fractional derivative was an ongoing topic for more than 300 years. Many noted mathematicians contributed to this theory over the years, among them Liouville, Riemann, Weyl, Fourier, Abel, Lacroix, Leibniz, Grünwald and Letnikov. Only in the last few decades, however, did applied scientists and engineers realize that such fractional differential equations provided a natural framework for the discussion of various kinds of questions modelled by fractional equations, such as viscoelastic systems, electrode-electrolyte polarization, colored noise, dielectric polarization, boundary layer effects in ducts, electromagnetic waves, quantitative finance, quantum evolution of complex systems, and fractional kinetics, etc. In this paper, we focus on studying fractional differential systems, where the fractional derivatives means the Caputo derivatives. Here we mainly prove local asymptotical stability of trivial solutions to the nonlinear fractional differential systems.

Time-step volume-preserving control of dissipative systems. **Jose-Manuel Zaldivar Comenges** (Joint Research Centre, Italy), Fernanda Strozzi (Università Carlo Cattaneo, Italy) IC/CT43/015

We present a general control and optimization strategy based on time-step state space volume preservation. This is performed by maintaining the divergence of the system close to zero. The on-line implementation is shown for batch and semibatch chemical reactors. The divergence of these reactors is reconstructed on-line using only reactor temperature measurements by applying state space reconstruction techniques. The simulated results for batch and semibatch processes are compared with a traditional control scheme. This approach allows, in addition to the process control, the optimization from performance and safety points of view.

On the Lyapunov-exponent spectrum. **Vladimir Dobrynskii** (National Academy of Sciences of Ukraine, Kyiv) IC/CT434/015

A fixed (periodic) point of map is asymptotic stable iff all its the Lyapunov exponents evaluated at the given point are negative. Transition of one the exponents through zero generates a bifurcation of phase pattern in the given point neighbourhood. There is a conjecture that an asymptotic stability and bifurcation of non-trivial topologically transitive subsets of map are connected with negativity of the Lyapunov exponents evaluated at all the subset points. The latter is a reason to study the Lyapunov exponent spectrum. We have the following rigorous mathematical results: (1) the most of piecewise lenear maps have continuous the Lyapunov exponent spectrum; (2) that of the logistic map is countable at the least.

IC/CTS4676/03: Simulation of biological systems.

Stability techniques in SIR epidemic models. **Zaman Khan** (Pusan National University Korea, Sud-Korea) IC/CT4322/003

The SIR models underestimates the variation in diseases spread, especially, if there is a lag between the infection of an animal and its own release of infectious material. Several strategies have been used to studied the SIR epidemic models. In this paper, we consider a nonlinear SIR model. The nonlinear system describing the dynamics of the interaction between susceptible and infected in population. We would like to analyze the dynamical behavior of nonlinear system and approach the system by stability techniques, to find the equilibrium positions of the susceptible population. We presented some mathematical models and discussed quantitatively to illustrate the solution of infected population.

Key words: Stability techniques, SIR model, Population

Global-attractivity conditions for single-species models. **Viktor Tkachenko** (National Academy of Sciences of Ukraine, Kyiv) IC/CT833/036

We consider the nonlinear difference equation with delay which arises in many contexts in mathematical biology

$$x_{n+1} = qx_n + f_n(x_n, ..., x_{n-k}), \quad n \in \mathbf{Z}, \qquad (1)$$

where $q \in (0,1]$ and functions $f_n : \mathbf{R^{n+1}} \to \mathbf{R}$ are estimated by a rational function $r(x) = ax/(1+bx)$, with $a < 0, b \geq 0$, such that $r(\mathcal{M}(\mathbf{z})) \leq f_n(\mathbf{z}) \leq r(-\mathcal{M}(-\mathbf{z}))$, where $\mathcal{M}(\mathbf{z}) = \max_i\{0, z_i\}$, the first inequality holds for all $\mathbf{z} \in \mathbf{R^{k+1}}$, and the second one for all $\mathbf{z} \in \mathbf{R^{k+1}}$ such that $\min_i z_i > -1/b$.

Treating eq. (1) as retarded differential equation with piecewise constant delays and applying our result for functional-differential equations we obtain

Theorem 1. If $q \in (0,1)$, $b \neq 0$ and the condition

$$q^{k+1} > -\frac{a}{1-q} \ln \frac{a^2 - a(1-q)}{a^2 + (1-q)^2},$$

holds, then $\lim_{n\to\infty} x_n = 0$ for every solution $\{x_n\}$ of Eq. (1).

In contrast to functional-differential equations this condition is not sharp within the class of difference equations (1).

Theorem 2. For every positive integer k there exists $q_k \in (0,1)$ such that for $q \in (0, q_k]$ the inequality

$$\frac{a}{1-q} \geq -\frac{1+q^{k+1}}{1-q^{k+1}} \qquad (2)$$

assures the global attractivity of eq. (1). Condition (2) is sharp within the class of described above eqs. (1) with $q \in (0, q_k]$.

We apply our results to discrete versions of NicholsonŠs blowflies equation, the Mackey-Glass equations, and the Wazewska and Lasota equation.

We give conditions for global attractivity of eq. (1) in the case $q = 1$ and show that these conditions are sharp if the equation is strongly non-autonomous. As application, we consider Ricker's equation with delayed-density dependence and generalization of the Pielou equation.

This is a joint work with Prof. Sergei Trofimchuk.

Mechanisms for oscillations in a biological competition model. **Rodica Curtu** (Transilvania University of Brasov, Romania) IC/CT839/033

In our work we analytically investigate a four-dimensional nonlinear dynamical system that models perceptual bistability in the brain. Perceptual bistability is a phenomenon reported in experiments when a subject is presented with ambiguous (visual) stimuli: for example, the subject's eyes are forced to 'see' two distinct images; as a result, the brain cannot deal with two percepts in the same place in space and at the same time, and an alternation between these occurs.

Two variables in the model correspond to the activity of each of the two competing units and they evolve in fast time; other two variables are slow and are associated with a negative feedback received by each unit separately. The main parameter took into consideration is the external input strength I.

We prove analytically that oscillations in the system appear through a supercritical Hopf bifurcation when the parameter I is decreased from large to moderate value. At lower values of I another Hopf bifurcation takes place and the limit cycle dissapears. Both normal form and bifurcation diagrams are constructed.

In addition, due to the presence of the two time-scales, in the range of I where oscillations exist, the limit cycle formed through the Hopf bifurcation tends rapidly to a relaxation-oscillator. We also characterize the system's behavior in this regime, giving a theoretical interpretation of what is observed in experiments.

Work done in collaboration with: John Rinzel and Asya Shpiro, New York University, USA

IC/CTS4659/03: Analysis and simulation.

Organiser: Nobusumi Sagara (Hosei University, Japan)

Binomial τ-leap spatial stochastic simulation algorithm. **Tatiana Marquez Lago** (University of Queensland, Australia), Kevin Burrage (University of Queensland, Australia) IC/CT518/012

In cell biology, cell-signaling pathway problems are often tackled with deterministic temporal models, well-mixed stochastic simulators and/or hybrid methods. But in fact, 3D stochastic spatial modeling of reactions happening inside the cell is needed in order to fully understand these cell signaling pathways. This is because noise effects, low molecular concentrations and spatial heterogeneity can all affect the cellular dynamics. However, there are ways in which important effects can be accounted without going to the extent of using highly-resolved spatial simulators (such as single-particle software), hence reducing the overall computation time significantly.

We present a new coarse grained modified version of the Next Subvolume Method, that allows the user to consider both diffusion and reaction events in relatively long simulation time spans as compared with the original method and other commonly used fully stochastic computational methods. Benchmarking of the simulation algorithm was performed through comparison with the Next Subvolume Method and well mixed models (Matlab), as well as stochastic particle reaction and transport simulations (ChemCell, Sandia National Laboratories).

Additionally, we consider a bi-stable system and construct a model based on a set of chemical reactions in the EGFR pathway. We analyse and outline the advantages of our presented Binomial τ-leap spatial stochastic simulation algorithm (τ-SSSA), in terms of efficiency and accuracy, in scenarios of both molecular homogeneity and heterogeneity.

Chaos in digital spaces. **Vinod Kumar Padingare Pisharathu Balakrishnan** (Rajagiri School of Engineering and Tech., India) IC/CT3857/035

Chaos in general topological spaces is widely studied. But in digital spaces $\mathbb{Z}2n$, with the usual topology it can be further explained. In this paper, we discuss chaos in $\mathbb{Z}2n$. The code space is the set of all words with infinite length in two symbols 0 and 1. It is a cantor set, so a fractal. We will show that in every digital space there exist at least one continuous function which is chaotic.

Representation of preference orderings on L^p-spaces by integral functionals: myopia, continuity and TAS utility. **Nobusumi Sagara** (Hosei University, Japan) IC/CT2354/030

The purpose of this paper is to present an axiomatic approach in a continuous time framework for representing preference orderings on L^p-spaces in terms of integral functionals. We show that if preference orderings on L^p-spaces satisfy continuity, separability, sensitivity, substitutability, additivity and lower boundedness, then there exists a utility function representing the preference orderings such that the utility function is an integral functional with an upper semicontinuous integrand satisfying the growth condition. Moreover, if the preference orderings satisfy the continuity with respect to the weak topology of L^p-spaces, then the integrand is a concave integrand. As a result, time additive separable (TAS) utility functions with constant discount rates are obtained.

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Existence of solutions for an eigenvalue problem. **Najib Tsouli** (Université Mohammed Premier Oujda, Morocco), Siham El Habib (University Mohamed I, faculty of sciences, Oujda, Morocco), Abdelrachid El Amrouss (Université Mohammed Premier Oujda, Morocco) IC/CT836/033

In this work we study the existence of solutions for the eigenvalue problem $\Delta_p^2 u = \lambda m(x)|u|^{p-2}u$, $u \in W^{2,p}(\Omega)$ in a bounded smooth domain Ω, with Neumann boundary condition $\frac{\partial u}{\partial \nu} = 0$ on $\partial\Omega$, and where $m \in L^r(\Omega)$, $m \neq 0$ is a weight function which can change its sign, with $r = r(N,p)$ satisfying the conditions: $r > N/2p$ for $N/p \geq 2$ and $r = 1$ for $N/p < 2$.

Some geometric properties of a Banach sequence space $m(\phi,p)$ related to l_p. **Mohammed Mursaleen** (Aligarh Muslim University, India) IC/CT2606/034

Let C denote the space whose elements are finite sets of distinct positive integers. Given any element σ of C, we denote by $c(\sigma)$ the sequence $\{c_n(\sigma)\}$ which is such that $c_n(\sigma) = 1$ if $n \in \sigma$,and $c_n(\sigma) = 0$ otherwise. Further

$$C_s = \Big\{\sigma \in C : \sum_{n=1}^{\infty} c_n(\sigma) \leq s\Big\},$$

the set of those σ whose support has cardinality at most s, and

$$\Phi = \Big\{\phi = \{\phi_n\} \in \ell^0 : \phi_1 > 0, \Delta\phi_k \geq 0 \text{ and } \Delta\Big(\frac{\phi_k}{k}\Big) \leq 0 \text{ for } (k = 1,2,\ldots)\Big\},$$

where $\Delta\phi_n = \phi_n - \phi_{n-1}$.
For $\phi \in \Phi$, we define the following sequence space, introduced by W.L.C. Sargent[1].

$$m(\phi) = \Big\{x = \{x_n\} \in \ell^0 : \sup_{s\geq 1} \sup_{\sigma\in C_s} \Big(\frac{1}{\phi_s} \sum_{n\in\sigma} |\, x_n \,|\Big) < \infty\Big\}.$$

It is easy to see that the space $m(\phi)$ is a Köthe sequence space, indeed a BK-space with respect to its natural norm.

In[2] Malkowsky and Mursaleen have characterized the matrix classes $(X, m(\phi))$ for any FK-space X. Recently some of the geometric properties of $m(\phi)$ have been investigated[3]. In this paper we extend the space $m(\phi)$ to $m(\phi,p)$ as follows and study its relations with the classical sequence space l_p and some of its geometric properties (e.g., ordered continuity, Fauto's property, Banach–Saks property, fixed-point property, Schur property etc.).

$$m(\phi,p) := \Big\{x = \{x_n\} \in \ell^0 : \sup_{s\geq 1} \sup_{\sigma\in C_s} \frac{1}{\phi_s} \sum_{n\in\sigma} |x_n|^p < \infty\Big\}.$$

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IC/CTS4665/03: Applied analysis for differential systems.

Organiser: Maxim Shamolin (Moscow State University, Russian Federation)

Periodic orbits in billiard systems. **Vadim Zharnitsky** (Univ. of Illinois at Urbana-Champaign, USA) IC/CT2846/030

The study of large sets (having positive measure) of periodic orbits in Birkhoff billiards is a classical problem in Hamiltonian dynamics. This problem is also important for the spectral asymptotics of the corresponding quantum mechanical system. It has been known that 2 and 3 period orbits constitute the set of zero measure in a Birkhoff billiard. We will describe a recently developed new approach to this problem relying on exterior differential systems and we will prove that the set of 4-period orbits in the smooth convex outer billiard (dual analog of Birkhoff billiard) has an empty interior.

On the Lagrangian formulation of a Lane–Emden-type equation and double reduction. **Chaudry Khalique** (North West University, South Africa) IC/CT4398/033

We classify the Noether point symmetries of the Lane–Emden-type equation $xy'' + ny' + x^\nu f(y) = 0$, for $\nu \neq 1$ with respect to the standard Lagrangian $L = \frac{1}{2}x^n y'^2 - x^{\nu+n-1}\int f(y)\,dy$ for various functions $f(y)$. We then obtain first integrals of the various cases which admit Noether point symmetry. Moreover, we find reduction to quadratures for the cases that admit Noether symmetries. Eight cases arise for the function $f(y)$ out of which seven cases result in Noether point symmetries.

Generalized de Rham–Hodge complexes, the related characteristic Chern classes and some applications to integrable multi-dimensional differential systems on Riemannian manifolds. **Anatoliy Prykarpatsky** (WMS AGH/IAPMM, Poland), Nikolay Bogolubov (jr.) (MI Russian Academy of Science) IC/CT936/034

The differential-geometric aspects of generalized de Rham–Hodge complexes naturally related with integrable multi-dimensional differential systems of M. Gromov type, as well as the geometric structure of Chern characteristic classes are studied. Special differential invariants of the Chern type are constructed, their importance for the integrability of multi-dimensional nonlinear differential systems on Riemannian manifolds is discussed. An example of the three-dimensional Davey–Stewartson type nonlinear strongly integrable differential system is considered, its Cartan type connection mapping and related Chern type differential invariants are analyzed.

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Predictive differential equations. **Toru Ohira** (Sony CSL, Tokyo, Japan) IC/CT1875/015

We study a system whose dynamics are governed by predictions of its future states. In particular, the following type of equations are discussed,

$$\frac{dx(t)}{dt} = -\alpha x(t) + f(\bar{x}(\bar{t})), \quad \bar{x}(\bar{t} = t + \eta) = \eta \frac{dx(t)}{dt} + x(t),$$

with constants $\alpha > 0$, and a parameter $\eta > 0$, called *advance*. As shown here, we assume that the current rate of change of x continues for the duration of the advance to estimate the future state of x. This is a common prediction scheme for population projections, the national debt estimations and so on, and termed as *fixed rate prediction*.

We find that the increasing value of η, indicating how far ahead in time to make a prediction, can induce rather complex behaviors to otherwise simple dynamics with a stable fixed point when $\eta = 0$. This characteristics is similar to those found with delay differential equations with increasing delay. Hence, we discuss the comparison of this type of equations with delay differential equations, both of them are incorporating non-locality on the time axis.

We also report that an added noise can induce a behavior similar to *stochastic resonance* with a tuned combination of the noise strength and advance. We refer to this effect as *predictive stochastic resonance*.

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4D rigid body and some cases of integrability. **Maxim Shamolin** (Moscow State University, Russian Federation) IC/CT3863/033

A mathematical model is constructed describing the deceleration of a solid 2D-, 3D- and 4D-body moving in a medium with a jet flow around the body in fore-dimensional space. The regime of translational deceleration is shown to be normally unstable. This has made it possible to develop a relatively simple technique for determining model parameters experimentally. An example of the application of this technique to a cylindrical body is presented.

The deceleration problem turned out to be more convenient for checking the build-up effect by experiment. The present study made it possible to develop a fairly simple and efficient technique for determining the unknown parameters of the model. Statement of a problem about the motion of a rigid body in a resisting medium when all the conditions of jet or separated flow are satisfied is given. This interaction of a medium with a body is concentrated on that part surfaces of a body, which has the form of a flat 1D- (cut), 2D- (circle) and 3D-disk.

At formation of dynamic model of influence of a medium on a 2D-, 3D- and 4D-body some properties of a medium are marked and its have connected in a serie of hypothesises. And the basic hypothesis is a hypothesis of quasistationarity. In this connection complete dynamic system describing investigated model is shown. Such class of motions which allow some constrain is considered. That constrain is allowing to consider some quantity as a constant in all time of a motion. That quantity is size of velocity of some characteristic point of a rigid body. The qualitative analysis of dynamic system obtained in space of quasivelocities is presented and it is recognized all the non-linear non-trivial properties.

Effective matrix formalism for singularity analysis of differential equations and new intergrable system in nonlinear elasticity. **Lydia Novozhilova** (Western Connecticut State University, USA), Sergei Urazhdin (West Virginia University, USA) IC/CT2702/030

New matrix formalism for finding series solutions to differential equations, developed by the authors earlier, and its extension to singularity analysis of ODEs and PDEs is presented.

Representing a power series as a product of two vectors

$$[a_0, a_1, a_2, \ldots] \cdot [1, x, /1!, x^2/2!, x^3/3!, \ldots]^T \qquad (1)$$

translates operations with analytic functions (like differentiation, multiplication by the independent variable, product of two such functions) into simple algebraic operations on the coefficient vectors and makes implementation of a classic power series method, even in the case of linear equations, elegant and simple. Using (1), a special matrix for computing the coefficient vector of the composite of two analytic functions can be defined, and information about the structure of this matrix can be pre-computed, stored, and used when needed. Using this universal matrix, nonlinear equations can be solved by

the power series method in the same simple and transparent manner as in the linear case. The extension of this formalism to the singularity analysis for differential equations with nonlinearity term given by analytic function is presented. The advantages of the approach are demonstrated on test problems (Burger's, KdV, Henon-Heiles equations). An example of new integrable system in nonlinear elasticity found by this method is also given.

IC/CTS4681/03: Bifurcation.

Organiser: Jan Sieber (University of Aberdeen, UK)

On the bandcount adding *bifurcation scenario.* **Viktor Avrutin** (Universität Stuttgart, Germany), Michael Schanz (Universität Stuttgart, Germany) IC/CT2416/035

An aperiodic and especially a chaotic attractor may consist of some number $K \geq 1$ of bands (also denoted as connected components). Multi-band chaotic attractors (MBCAs) defined by the bandcount $K > 1$, represent a well-known phenomenon on the field of nonlinear dynamics and are often involved in several bifurcations. It is for instance well-known, that the period doubling cascade is typically followed by an inverse band merging cascade, which represents a sequence of MBCAs with $p_0 \cdot 2^n$ bands, whereby n decreases from infinity to zero. We report a novel bifurcation scenario (bandcount adding scenario), which involves an infinite number of MBCAs organized not sequentially, but according to an infinite adding scheme. This adding scheme which is similar to the well-known Farey-trees, implies that between two MBCAs with bandcounts K_1 and K_2 there is an MBCA with $K_1 + K_2 - K^0$ bands (with some constant offset K^0). This scenario continues ad infinitum and resembles the period adding scenario known from many applications, but in contrast to this is formed by chaotic and not by periodic attractors. We study this scenario using a discontinuous map, which is actually considered by many authors as some kind of normal form of the discrete-time representation of many non-smooth systems of practical interest in the neighborhood of the point of discontinuity. By investigation of the structure of the 2D parameter space, we find out, that the bandcount adding scenario is related with discontinuity-induced codimension-1 bifurcations of unstable periodic orbits and with some specific discontinuity-induced codimension-2 bifurcations. Consequently, we describe the self-similarity of the chaotic area in parameter space and show, that in this area there are much more non-robust chaotic attractors than typically assumed.

On some generic types of discontinuity induced codimension-3 bifurcations. **Michael Schanz** (Universität Stuttgart, Germany), Viktor Avrutin (Universität Stuttgart, Germany) IC/CT2450/015

In this work we consider two families of piecewise-linear maps with a discontinuity, which is motivated by modeling of several power electronic circuits (DC/DC converters, Sigma-Delta modulators) and which is already investigated by many authors. However, the focus of these works lie on the investigation of the dynamics by variation of one or at most two system parameters. In many of these publications a great variety of bifurcation phenomena is revealed but unfortunately, a profound explanation of the complicated and often self-similar bifurcation structures and the systematics behind is missing.

In contrast to that, we investigate the full 3D parameter space of these families of systems and detect a number of discontinuity induced codimension-3 bifurcations. Some of them belong to an already known generic type [1,2], while others represent some new types not investigated so far.

Unfolding these bifurcations we are able to explain the systematics for a large number of the above mentioned bifurcation phenomena. In particular, several bifurcation scenarios observed under variation of one or two parameters represent an intersection of the extended bifurcation structures induced by codimension-3 bifurcation with the corresponding 1D or 2D parameter subspace.

The codimension-3 bifurcations reported here are characterized by two manifolds in the 3D parameter space, a 1D and a 2D one. The 1D manifold represents a codimension-2 bifurcation curve, whereas in the 2D manifold an infinite number of codimension-2 bifurcation curves are located. At the codimension-3 bifurcation point all these curves intersect. The reported bifurcations serve as organizing centers of periodic and aperiodic dynamics in the overall parameter space.

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Neimark–Sacker Hopf bifurcations and snap-back repellers for the modified Nicholson–Bailey model. **Chen-Chang Peng** (No.300 Syuefu Rd., Chiayi City 60004, Taiwan) IC/CT3427/036

In this talk, we study the modified Nicholson-Bailey model with one parameter.

$$(x, y) \longmapsto (xe^{[3(1-x)-\alpha y]}, x(1 - e^{-\alpha y}))$$

Based on the bifurcation diagram versus parameter $\alpha \in (3.2, 3.3)$, we realize that a Neimark-Sacker Hopf bifurcation takes place at $\alpha = \alpha^* \in (3.2, 3.3)$. We hence investigate a rigorous proof of the existence of the Neimark-Sacker Hopf bifurcation. For each $\alpha \in (4.3, 5.8)$ we present a computer-assisted method to prove rigorously that the existence of snapback repellers for this model and hence it has chaotic behavior for each $\alpha \in (4.3, 5.8)$.

Control-based bifurcation analysis. **Jan Sieber** (University of Aberdeen, UK), Yuliya Kyrychko (University of Bristol, UK) IC/CT3141/033

We introduce a method for tracking nonlinear oscillations and their bifurcations in nonlinear dynamical systems. Our method does not require a mathematical model of the dynamical system nor the ability to set its initial conditions. Instead it relies on feedback stabilizability, which makes the approach applicable in experiments. The main area of application for this method are stability tests in civil and mechanical engineering that couple mechanical experiments and computer simulations, so-called hybrid, or substructured, tests. We will demonstrate our method using a simple hybrid system, consisting of a periodically forced mass-spring-damper (which is simulated in the computer) and a pendulum (which is real, and coupled to the simulation via actuators). Proof-of-concept computer simulations, including adverse effects such as coupling delay and measurement inaccuracies, have been successful. The incorporation of control-based bifurcation analysis into the hybrid experiment itself is currently in preparation.

Period-doubling cascades and mode interactions in coupled systems. **Philip Aston** (University of Surrey, UK) IC/CT1427/034

Suppose that an iterated map exhibits a period-doubling cascade. If two such maps are coupled, then the synchronised state will exhibit the same period-doubling cascade but there is also the additional possibility of symmetry-breaking bifurcations to non-synchronised states. By introducing a second parameter, a symmetry-breaking bifurcation and a period-doubling bifurcation can be made to occur at the same point, resulting in a mode interaction.

As the second parameter is varied from the value at the mode interaction, a second symmetry-breaking bifurcation may occur from the period 2 solutions, which will then be involved in another mode interaction at the next period-doubling bifurcation point. In this way, a complete cascade of mode interactions can occur.

A local analysis of such a mode interaction is performed. The global consequences together with a classification of different cases are then considered. Renormalisation theory is used to determine the universal behaviour and parameter scalings of such a system.

This work is done in collaboration with Himat Mir.

Self-oscillations in a system of regulation with hysteresis in the source therm. **Arzigul Shayakhmetova** (MIRAS University, Kazakhstan) IC/CT4559/033

For the parabolic system of regulation of temperature the questions of existence and uniqueness of periodical solutions are considered. It is formulated conditions of existance such kind of solutions and found estimates for periods of the self-oscillations. Hysteresis condition is on a boundary. Regulation condition is a linear continuous non-negative functional in C[0,1] or in L2(0,1), such that in C[0,1] the temperature is regulated in a fixed point, in L2(0,1) is regulated at an average temperature. Considered system has two parameters - the temperature of switching on and the temperature of switching off, influenced by periods of self-oscillations.

IC/CTS4669/03: Nonlinear PDEs and ODEs, oscillations.

Organiser: Eugene Starostin (University College London, UK)

Coupled-cell systems: a paradigm for developing advanced magnetic sensors. **Antonio Palacios** (San Diego State University, USA) IC/CT1770/033

A large class of dynamic sensors exhibit nonlinear input-output characteristics, often corresponding to a bistable potential energy function. Examples include: magnetic field sensors, e.g., fluxgate sensors, ferroelectric sensors, and mechanical sensors, e.g., acoustic transducers made with piezoelectric materials. Many of these sensors have assisted mankind in analyzing and controlling thousands of functions for many decades. Computer memory has increased over many years through the use of magnetic sensors embedded in storage devices. Airplanes fly with higher safety standards because of the high reliability of noncontact switching with magnetic sensors. As new technologies emerge, however, more powerful and more efficient sensors are required.

Using ideas and methods from nonlinear dynamics research (in particular bifurcation theory) in Engineering, Mathematics, and Physics, we present theoretical and experimental results which demonstrate that higher sensitivity, lower power-consumption, and reduced costs, can all be achieved through an integrative approach that combines a novel Intelligent Magnetic Sensor (IMS) network architecture with a new read-out technique, the Residence Time Detection (RTD). The IMS/RTD concept is device-independent, so that similar principles can be readily adapted to a wide variety of sensors. In this work, we will consider, in particular, fluxgate magnetometers, Superconducting Quantum Interference Devices, and electric-field sensors. The research work is part of an ongoing collaboration between the Nonlinear Dynamical System group at San Diego State University and the Applied Chaos and Dynamics program at the Space and Naval Warfare Center in San Diego.

The dynamics of wheel shimmy with delay and tyre relaxation length. **Gábor Orosz** (University of Exeter, UK), Dénes Takács (Budapest University of Technology and Economics, Hungary), Gabor Stepan (Budapest University of Technology and Economics, Hungary) IC/CT1798/033

Lateral vibrations of wheels, the so-called the shimmy motion, may appear on airplane landing gears and motorcycle wheels and also on wheels of semi-trailers or articulated buses presenting a safety hazard. The nonlinear dynamics of shimmy is studied when the vibrations are due to the elasticity of the tyre. We consider the case when the wheel is pulled by a caster with constant velocity. The lateral deformations of the tyre are modelled by a stretched string model: the tyre ground contact is considered as a contact line which becomes deformed due to the lateral displacement of the wheel. Furthermore, we assume that each contact point sticks to the ground that results in a non-holonomic constraint expressed by a first order partial differential equation (PDE). With the appropriate choice of the boundary conditions, the so-called relaxation length of the tyre is also taken into account among other conventional tyre parameters like the specific stiffness and damping. The equation of motion is an integro differential equation (IDE). Assuming travelling wave solutions of the deformation allows us to transform the (PDE-IDE) system into a delay differential equation (DDE) with distributed delay. Here, the delay is the time needed for the leading point of the contact line to travel backward (relative to the caster) to the considered contact point. The linear stability investigation of the DDE shows that the steady rolling motion may loose its stability via codimension-one or codimension-two Hopf bifurcations as the parameters (like the towing speed and the caster length) are varied. Consequently, self-excited periodic and quasi-periodic oscillations can appear. The stability chart in the plane of the above parameters is determined semi-analytically, and also checked experimentally. The results confirm the importance of the relaxation length parameter in the model. Our results may help designers to eliminate this unwanted phenomenon.

Coupling and noise-induced patterns on $O(2)$ symmetric domains. **Peter Blomgren** (San Diego State University, USA) IC/CT2791/033

We study the Kuramoto–Sivashinsky equation, an example of a temporally pattern-forming dynamical system with a two-dimensional circular domain. Numerical integration of the pure KS equation leads to predominantly static cellular patterns. The introduction of additive noise (modeling thermal fluctuations), or parametric noise (modeling fluctuations in the physical control parameters) greatly increases the propensity of dynamic cellular states, which seems to explain the generic behavior of related laboratory experiments. Further, coupling to the heat equation (modeling interaction with the combustion chamber), gives rise to additional dynamic patterns. We report on the numerical simulation and analysis of recently found dynamic patterns, including modulated rotations, hopping, and homoclinic intermittent states. Many of these states were previously only observed in physical experiments or, in some cases, predicted by bifurcation analysis.

Regularity and determining modes for partly-dissipative reaction–diffusion systems. **Zhoude Shao** (Millersville University, USA) IC/CT1468/033

We consider an abstract system of evolutionary equations of the form

$$\begin{cases} u' + Au = F(u,v) \\ v' + B(u)v = G(u,v) \end{cases} \quad (1)$$

on a Hilbert space $H_1 \times H_2$, where A is a linear unbounded positive self-adjoint operator with a compact resolvent on H_1 and $B(u)$ is a linear bounded positive operator on H_2. Assume that system (1) possesses a global attractor (or more generally, a compact invariant set). Sufficient conditions are given to guarantee the smoothness of solutions of (1) on the global attractor. Also derived are results related to determination of solutions of system (1) by finitely many determining modes, the eigenfunctions of the operator A. The results obtained represent generalizations of the corresponding results by Hale and Raugel (J. Math. Pures Appl. (9)82 (2003)). Applications of these abstract results are given to partly dissipative reaction diffusion systems and systems admitting invariant regions which include the FitzHugh-Nagumo equations and Hodgkin-Huxley equations as examples.

Motion of polygonal curves by crystalline curvature flow and its generalization. **Tetsuya Ishiwata** (Gifu University, Japan) IC/CT1636/033

We discuss a motion of polygonal curves in the plane by crystalline curvature flow $V_j = H_j$ and its generalization $V_j = g(\theta_j, H_j)$. Here V_j, θ_j and H_j denote a normal velocity, a normal angle and a crystalline curvature of j-th edge of solution polygon, respectively. We consider the solution curves in the special class of polygonal curves which is characterized by an interfacial energy density. We call this class *admissible class*. In this talk, we show that (i) the solution polygon belongs to the admissible class as long as the solution exists, (ii) a crystalline curvature of each edges becomes non-negative before the extinction time and (iii) the solution polygon becomes star-shaped before the extinction time under some assumptions.

The equilibrium shape of an elastic developable Möbius strip. **Eugene Starostin** (University College London, UK), Gert van der Heijden (University College London, UK) IC/CT2500/015

The Möbius strip, obtained by taking a rectangular strip of plastic or paper, twisting one end through 180°, and then joining the ends, is the canonical example of a one-sided surface. As simple experimentation shows, a physical Möbius strip, when left to itself, adopts a characteristic shape independent of the type of material (sufficiently stiff for gravity to be ignorable).

This shape is well described by a developable surface that minimises the deformation energy, which is entirely due to bending. We assume that the material obeys Hooke's linear law for bending, then the energy is proportional to the integral of the non-zero principal curvature squared over the surface of the strip, which is taken to be an isometric embedding of a rectangle into 3D space.

The problem of finding the equilibrium shape of narrow Möbius strip was first formulated by M. Sadowsky in 1930 who turned it into a 1D variational problem represented in a form that is invariant under Euclidean motions. Later W. Wunderlich generalised this formulation to a strip of finite width, but the problem has remained open although *geometrical* constructions of developable Möbius strips have appeared.

We apply an invariant geometrical approach based on the variational bicomplex formalism to derive the first equilibrium equations for a finite-width developable strip thereby giving the first non-trivial demonstration of the potential of this approach. The boundary-value problem for the Möbius strip offers a fitting example for application of these equations.

Numerical solutions for increasing width-to-length ratio show the formation of creases bounding nearly flat triangular regions, a feature also familiar from fabric draping and paper crumpling. This suggests that our approach could give new insight into energy localisation phenomena in unstretchable elastic sheets, which for instance could help to predict points of onset of tearing.

IC/CTS4662/03: Integrable systems, solitons, control theory.

Organiser: Balachandran Krishnan (Bharathiar University, Coimbatore, India)
Co-organiser: Nagarajan Sukavanam (IIT Bombay, India)

Exact controllability of semilinear thermoelastic system with control and non-linearity in thermal component only. **Nutan Tomar** (IIT Roorkee, India), Nagarajan Sukavanam (IIT Bombay, India) IC/CT3556/030

In this paper, we are concerned with the study of exact controllability of a semi-linear thermo-elastic system described by the partial differential equations:

$$\omega_{tt} - \gamma\Delta\omega_{tt} + \Delta^2\omega + \alpha\Delta\theta = 0 \text{ in } \Omega_T \quad (1a)$$

$$\theta_t - \Delta\theta + \sigma\theta - \alpha\Delta\omega_t + g(\omega) = u \text{ in } \Omega_T \quad (1b)$$

with Dirichlet boundary conditions and given initial conditions. Here Ω is a bounded open subset of R^2 with smooth boundary and $\Omega_T = \Omega \times (0,T)$, where $T > 0$ is the final time at which we want to achieve the controllability. The non-linearity is due to the non-linear function g, and u is the control function which acts only on the equation (1 b). The system (1) without the control and non-linear function g is a partial differential equation model which describes a Kirchhoff plate subjected to a thermal damping. Here ω is the displacement θ is the temperature of the plate and $\alpha > 0, \gamma \geq 0, \sigma \geq 0$ are the given system parameters.There is a vast amount of literature with various types of controllability of linear systems (i.e. $g = 0$) similar to (1) with the controls either as distributed controls or through the boundary. It has been proved in recent litrature that if the lipschitz constant of g is sufficiently small, then the semilinear system is exact controllable. In this paper, we removed the condition that lipschitz constant is sufficiently small for the exact controllability of system (1).

Approximate controllability of abstract semilinear control systems. **Nagarajan Sukavanam** (IIT Bombay, India), Divya Divya (IIT Roorkee, India) IC/CT3634/030

In this paper we prove the approximate controllability (a.c) of semilinear control systems of the form

$$x_u'(t) = Ax_u(t) + Bu(t) + f(t, x_u(t)); 0 \leqslant t \leqslant T \quad (1a)$$

$$x_u(0) = 0 \quad (1b)$$

where the state $x_u(t)$ of the system takes values in a Hilbert space V and the control function $u(t)$ takes its values in the Hilbert space $\hat{V}$. Let $Z = L_2[0,T;V]$ and $Y = L_2[0,T;\hat{V}]$ be the function spaces corresponding to V and $\hat{V}$ defined on $[0,T]$. Here, $B : Y \to Z$ is a bounded linear operator , $f : [0,T] \times V \to V$ is a non linear operator, $A : D(A) \subset V \to V$ is a closed operator whose domain $D(A)$ is dense in V. The system (1) is said to be a.c. in the time interval $[0,T]$, if for every desired final state $x_T \in V$ and $\varepsilon > 0$ there exists a control function $u \in Y$, such that the solution $x_u(\cdot)$ of (1) satisfies $\| x_u(T) - x_T \| < \varepsilon$. In controllability literature, it is common to use Fixed point or De-

gree theory argument to establish a.c of the above semilinear control system, which makes it necessary to assume certain inequality conditions involving various system constants. These conditions are often difficult to verify for a given system. In this paper the a.c is proved using a direct approach, avoiding fixed point arguments for certain class of nonlinear functions f. The main assumption on f is that it satisfies negative monotonicity.

Controllability of neutral functional evolution integrodifferential systems with infinite delay. **Balachandran Krishnan** (Bharathiar University, Coimbatore, India) IC/CT4115/030

In this paper we establish a set of sufficient conditions for the controllability of neutral functional evolution integrodifferential systems in Banach spaces. This class of neutral equations serve as an abstract formulation of many partial neutral integrodifferential equations which arise in the applications of the theory of population dynamics, compartmental systems, viscoelasticity and many other fields of science. The controllability results are obtained by using the analytic semigroup theory and the Nussbaum fixed point theorem.

Carleman estimate for parabolic equation with memory effects and exact controllability. **Sakthivel Kumarasamy** (Bharathiar University, India) IC/CT1053/062

The result of this work concerns with the exact controllability to the trajectories for a nonlinear parabolic equation with memory effects of the form

$$y_t - \mu y_{xx} + y y_x - \int_0^t k(t-\tau) y_{xx}(\tau) d\tau = \chi_\omega(x) u \quad \text{in } (0,T)\times\Omega$$

with the homogeneous Neumann boundary data

$$\frac{\partial y}{\partial \nu} = 0 \quad \text{on } (0,T)\times\partial\Omega, \quad y(0,x) = y_0(x) \quad \text{in } \Omega,$$

where Ω is a nonempty open bounded and connected subset of $\mathbb{R}$ with smooth boundary $\partial\Omega$ of class C^2 and ν is the outword unit normal vector to the boundary $\partial\Omega$. Here $\mu > 0$ is a constant, χ_ω is the characteristic function of the open set $\omega \subset \Omega$, $y = y(t,x)$ is the state and $u = u(t,x)$ is the control function to be determined which acts on the system through ω. This model arises in a number of practical applications, for example, in the modeling of physical phenomena associated with heat flow in materials with memory and the models involving viscoelastic forces.

The proof relies on Kakutani's fixed point theorem and makes use of the null controllability results for the corresponding linearized system (with $\mu = 1$)

$$y_t - y_{xx} + a(t,x) y_x + b(t,x) y - \int_0^t k(t-\tau) y_{xx}(\tau) d\tau = \chi_\omega(x) u.$$

Here it is assumed that the coefficients a, b and the kernel k satisfy

$$a \in L^\infty((0,T)\times\Omega), \quad b \in L^\infty((0,T)\times\Omega) \quad \text{and} \quad k \in C^1[0,T], \quad k(0) = 0.$$

The global exact null controllability results for the above linear parabolic equation with memory is established as the limit of an approximation process, constructed with the aid of a family of optimal control problem for the linear system and the observability estimate which is the consequence of a Carleman inequality for the associated adjoint system.

Robust controllability of linear systems: analysis and application to pursuit problems. **Valery Glizer** (Technion – Israel Institute of Technology), Vladimir Turetsky (Technion – Israel Institute of Technology) IC/CT1352/030

Controllability, i.e. the ability to transfer a dynamic system from a given set of initial positions to a given target set by a proper choice of the control function, is one of the basic system properties. Controllability has been well studied for systems without uncertainties by using an open-loop control.

Unfortunately, this elegant theory is not always applicable to real-life systems because their dynamics is effected by unmeasurable components (uncertainties). For these systems, the controllability, robust with respect to any admissible uncertainty realization, should be studied. As a rule, the robust controllability is realized by a feedback control.

In this talk, a class of linear time-dependent controlled systems with additive input uncertainties (disturbances) is considered. The target set is a given linear manifold. For this system, necessary and sufficient robust controllability conditions are established.

It is important not only to know that a system is robustly controllable, but also to construct a proper class of feedback strategies realizing this controllability (transferring strategies). In this talk, a class of linear state-feedback transferring strategies is derived.

The general robust controllability concept does not take into account possible control constraints, although such constraints are indispensable part of most of practical control problems. Thus, the next step is to adapt the results on the robust controllability to the case of control constraints. This leads to the constructing a robust controllability set, i.e. the set of all initial positions, from which the robust transfer of the system to the target set is possible subject to the control constraints.

The theoretical results of this talk are applied to some pursuit problems arising in the aerospace engineering.

Complete controllability of perturbed stochastic integro-differential systems. **Karthikeyan Shanmugasundaram** (Bharathiar University, India) IC/CT4120/030

In this paper we examine the controllability of a semilinear stochastic integrodifferential system in finite dimensional spaces. This type of equations occur in population models where the integral term specifies how much weight attached to the population at varies past times, in order to arrive at their present effect on the resources availability. The complete controllability of such equations is of quite fundamental importance biologically when the parameters are subject to some random disturbances like environmental factors. The study of this phenomena has become an essential part of qualitative theory of stochastic differential equations. The results are obtained by using the Banach fixed point theorem and an example is provided to illustrate the technique.

IC/CTS4673/03: Nonlinear PDEs and ODEs, oscillations.

Organiser: Nikolaos Stavrakakis (National Technical University of Athens, Greece)
Co-organiser: Richard Haberman (Southern Methodist University, USA)

Existence and uniqueness results for a nonlinear differential system. **Rodica Luca-Tudorache** (Technical University of Iaşi, Romania) IC/CT523/033

We investigate the existence, uniqueness and asymptotic behaviour of the strong and weak solutions to the nonlinear differential system

$$u_j'(t) + \frac{v_j(t)-v_{j-1}(t)}{h_j} + c_j A(u_j(t)) \ni f_j(t)\,,$$
$$v_j'(t) + \frac{u_{j+1}(t)-u_j(t)}{h_j} + d_j B(v_j(t)) \ni g_j(t)\,,$$

where $j = \overline{1,N}$, with $t \in [0,T]$ in H, with the boundary condition:

$$(v_0(t), -u_{N+1}(t), s_1 w_1'(t), \dots, s_m w_m'(t))^T \in$$
$$\in -\Lambda((u_1(t), v_N(t), w_1(t), \dots, w_m(t))^T),\ t \in [0,T]$$

and the initial data

$$u_j(0) = u_{j0}\,, \quad v_j(0) = v_{j0}\,, \quad j = \overline{1,N}$$
$$w_i(0) = w_{i0}\,, \quad i = \overline{1,m}\,,$$

where H is a real Hilbert space, $N \in \mathbb{N}$, $T > 0$, c_j, d_j, $h_j > 0$, $\forall j = \overline{1,N}$, and A, B are multivalued operators in H and Λ is a multivalued operator in H^{m+2}, which satisfy some assumptions.

This problem is a discrete version with respect to x (with $H = \mathbb{R}$) of some problems which have applications in integrated circuits modelling (see [4-6]), and it is a generalization of the case studied in [3]. For the proofs of our theorems we use several results from the theory of monotone operators and nonlinear evolution equations of monotone type in Hilbert spaces (see [1-2]).

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A continuation method for positive bound state of N coupled nonlinear Schrödinger equation. **Yuen-Cheng Kuo** (National University of Kaohsiung, Taiwan) IC/CT1394/033

We develop a stability continuation method for the computation of positive bound states of time-independent, N coupled nonlinear algebra equation (NAE) which describe a N coupled nonlinear Schrödinger equation. The solution curve with respect to some parameter of the NAE is then followed by the proposed method. For a one component NAE, we develop a iterative method for computation of positive ground state solution. For a N coupled NAE, we prove that N identical positive bound states will bifurcate into N different positive bound states at a finite repulsive inter-component scattering length. Numerical results show that various positive bound states of a three-component NAE are solved efficiently and reliably by the continuation method.

Multiplicity results for quasi-linear problems. **Abdelrachid El Amrouss** (Université Mohammed Premier Oujda, Morocco) IC/CT886/033

Let us consider the nonlinear elliptic problem

$$(\mathcal{P}) \begin{cases} -\Delta_p u = f(x,u) & \text{in } \Omega, \\ u = 0 & \text{on } \partial\Omega, \end{cases}$$

where Ω is a bounded domain in $\mathbb{R}^N$ with smooth boundary $\partial\Omega$, Δ_p is the p-Laplacian operator defined by $\Delta_p u := div(|\nabla u|^{p-2}\nabla u)$, $1 < p < \infty$ and $f : \Omega \times \mathbb{R} \to \mathbb{R}$ is a Carathéodory function satisfying the subcritical growth

$$(f_0) \qquad |f(x,t)| \le c(1+|t|^{q-1}),\ \forall t \in \mathbb{R},\ \text{a.e x} \in \Omega,$$

for some $c > 0$, and $1 \le q < p^*$ where $p^* = \frac{Np}{N-p}$ if $1 < p < N$ and $p^* = +\infty$ if $N \le p$.

Applying an minimax arguments and Morse theory, we establish some results on the existence of multiple nontrivial solutions for a problem $\mathcal{P}$.

Kink-antikink nonlinear-wave collisions in a cubic Klein-Gordon equation: the n-bounce resonance and the separatrix map. **Richard Haberman** (Southern Methodist University, USA) IC/CT4335/030

We provide a detailed mathematical explanation of a phenomenon known as the two-bounce resonance observed in collisions between kink and antikink traveling waves, originally extensively investigated in the 1980s by Campbell and his collaborators.. Studying a finite-dimensional "collective coordinates" model, we use geometric phase-plane based reasoning and matched asymptotic expansions to explain the mechanism underlying the phenomenon. We derive the critical relative velocity below which the interacting kinks have complex behavior and compare it to new high-resolution numerical simulations. We derive a separatrix map that explains the complex fractal-like dependence on initial velocity for kink-antikink interactions. Joint work with Roy Goodman.

Finite dimensionality of the global attractor for a Klein–Gordon–Schrödinger equation. **Nikolaos Stavrakakis** (National Technical University of Athens, Greece), Poulou Marilena (National Technical University of Athens, Greece) IC/CT4750/033

In this talk we prove the existence and uniqueness of solutions for the following evolution system of Klein–Gordon–Schrödinger type

$$\begin{aligned} i\psi_t + \kappa\psi_{xx} + i\alpha\psi &= \phi\psi + f, \\ \phi_{tt} - \phi_{xx} + \phi + \lambda\phi_t &= -Re\psi_x + g, \\ \psi(x,0) = \psi_0(x),\ \phi(x,0) &= \phi_0(x),\ \phi_t(x,0) = \phi_1(x), \\ \psi(x,t) = \phi(x,t) &= 0,\ x \in \partial\Omega,\ t > 0, \end{aligned}$$

where $x \in \Omega$, $t > 0$, $\kappa > 0$, $\alpha > 0$, $\lambda > 0$, f and g are driving terms and Ω (bounded) $\subset \mathbb{R}$. Next, with the help of the energy equation we prove that the solutions of the system depend continuously on the initial data and as a consequence the existence of a global attractor. Finally, the finite dimensionality of the global attractor is studied. Actually by means of the Lyapunov exponents we give an upper bound for the Hausdorff and Fractal dimensions of the global attractor.

This work was partially financially supported by a grant from the Pythagoras Basic Research Program No. 68/831 of the Ministry of Education of the Hellenic Republic.

Control of noise-induced behavior in neural network. **Natalia Janson** (Loughborough University, UK), Sandhya Patidar (Loughborough University, UK) IC/CT4713/033

We study the effect of time-delayed feedback control on the noise-induced dynamics [1] of an ensemble of N globally coupled excitable neural oscillators, each being modeled by the FitzHugh–Nagumo system with independent Gaussian white noise source. Both coupling and feedback are introduced through the mean field. The effect of delayed feedback is studied both analytically and numerically.

For the theoretical study we exploit a method of [2] introduced in [3], which allows one to write down a closed system of cumulant equations for the mean values, variances and covariances of the system variables, under the assumption that their third and higher order central moments are relatively small.

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IC/CTS4675/03: Model systems, diffusion, biological systems.

Organiser: Takeshi Sugimoto (Kanagawa University, Japan)

Bistable waves in discrete inhomogeneous media. **Brian Moore** (University of Iowa, USA), Antony Humphries (McGill University, Canada) IC/CT3186/036

Using a specific bistable nonlinearity for a spatially discrete Nagumo equation with inhomogeneous diffusion, one is able to derive explicit solutions by way of transform techniques and Jacobi operator theory. A topic of particular interest concerning this problem is the conditions that imply propagation failure of traveling wave solutions. By finding the steady state solutions, we derive necessary and sufficient conditions for traveling waves to become pinned due to variations in the diffusion coefficients.

On the structure of phase spaces in synergetic inter-representation network. **Takeshi Sugimoto** (Kanagawa University, Japan) IC/CT1051/036

Exchanging ideas and concepts among people can be handled with so-called Synergetic Inter-Representation Network. In this theory representations in our minds and outside ourselves constitute networks. The state in our mind, n-dimensional $\mathbf{x}$, is described by

$$\frac{\mathrm{d}\mathbf{x}}{\mathrm{d}t} = \sum_{j=1}^{n} \left\{ \lambda_j - B \sum_{i=1,\ i\neq j}^{n} \left(\mathbf{v}_i^+ \cdot \mathbf{x}\right)^2 \right\} \left(\mathbf{v}_j^+ \cdot \mathbf{x}\right) \mathbf{v}_j - C|\mathbf{x}|^2 \mathbf{x},$$

where λ_j, B, C, $\mathbf{v}_j$ and $\mathbf{v}_j^+$ denote the growth rate of the jth representation, the discrimination rate, the noise-eliminating rate, the jth representation and its adjoint, respectively. The adjoining order parameter, ξ_j, is defined by $\mathbf{v}_j^+ \cdot \mathbf{x}$. Multiplying the governing equation of ξ_j by ξ_j and rewriting ξ_j^2 as η_j, we obtain

$$\frac{\mathrm{d}\eta_j}{\mathrm{d}t} = 2 \left\{ \lambda_j - (B+C) \sum_{i=1}^{n} \eta_i + B\eta_j \right\} \eta_j \text{ for } j = 1, 2, \cdots, n,$$

that is, n-dimensional Lotka-Volterra equations. This discovery allows us to scrutinize the existence and stability of the fixed points: 1. The origin is an unstable fixed point; 2. The single representation survival, for example $(0, 0, \cdots, \lambda_j/C, \cdots, 0)$, is a stable fixed point, if $\lambda_j/C > \lambda_i/(B+C)$ for all $i \neq j$; 3. The coexistence of several representations, for example $(\eta_1, \eta_2, \cdots, \eta_k, 0, \cdots, 0)$, exists as a saddle point, if

$$\lambda_j < \frac{B+C}{(k-1)B + kC} \sum_{i=1}^{k} \lambda_i \text{ for } j = 1, 2, \cdots, k.$$

If all of these exist, the number of the saddle points is $2^n - n - 1$.

In the presentation, I will display the four-dimensional phase space and the high-dimensional separatrices using the directed graph.

Feedback control of pattern formation. **Liam Stanton** (Northwestern University, USA), Alexander Golovin (Northwestern University, USA) IC/CT1470/036

A global feedback control of pattern formation in a wide class of systems described by the Swift-Hohenberg (SH) equation is investigated theoretically, by means of stability analysis and numerical simulations. Two cases are considered: (i) feedback control of the competition between hexagon and roll (stripe) patterns described by a supercritical SH equation, and (ii) the use of feedback control to suppress the blow-up in a system described by a subcritical SH equation. In case (i), it is shown that feedback control can change the hexagon and roll stability regions in the parameter space as well as cause a transition from up- to down-hexagons and stabilize a skewed (mixed mode) hexagonal pattern. In case (ii), it is demonstrated that feedback control can suppress blow-up and lead to the formation of spatially-localized patterns in the weakly nonlinear regime. The effects of a delayed feedback are also investigated for both cases, and it is shown that delay can induce temporal oscillations as well as blow-up.

Creative brain neuron dynamics simulated by the discrete 2D and 3D space-distributed logistic equation. **Vladimir Gontar** (Ben-Gurion University, Israel) IC/CT4231/036

Mathematical modeling of the brains neurons networks by the interconnected oscillators with chaotic regimes is one of the effective methods to simulate brain creativity in a form of artistic 2D images within their relation to the brain waves (EEG) [1].In this work we would like to present some new results on creative patterning based on exploiting dynamics of interconnected chaotic oscillators distributes on 2D and 3D lattices (LxL)and (LxLxL) where each cell designated by the integer coordinates i,j,k =1,2,ĚL and contain discrete dynamical system (chaotic oscillator in a form of logistic equation)and for 2D case: Xn+1(i,j)= pn(i,j)Xn(i,j)(1-Xn(i,j). Here parameter pn (i,j) = F(b, Xn-1 (i,j)) depend on the values Xn-1(i,j) distributed on 2D lattice and calculated for the previous to n discrete states (n-1,n=1,2,...) In the simplest case Xn-1(i,j) just the closest to the considered cell with coordinates (i,j) eight neighbors with coordinates (i,j) = (i-1,j-1; i+1,j;Ěi+1,j+1),(for the 3D lattice: 26 neighbors), F is an arbitrary chosen analytical function with the parameters b. It will be shown that discrete logistic equation can be used for generating colored symmetrical patterns within the interval 3.57=pn(i,j)=4. Variety of the patterns resulted from the proposed approach can be drastically increased by using different functions F, varying the parameters b and by using other types of basic difference equations with chaotic regimes[2]. References:[1] Gontar, V. (2004), The dynamics of living and thinking systems, biological networks and the laws of physics, Discrete Dynamics in Nature and Society, 8 (1).[2] Gontar, V., Grechko, O. (2006), Generation of symmetrical colored images via solution of the inverse problem of chemical reactions discrete chaotic dynamics, Int. J. Bifurcation and Chaos, 16(5).

Controlling chaos in nuclear-spin generator system using back-stepping design. **Ömür Umut** (Abant Izzet Baysal University, Turkey) IC/CT4292/030

In this study, I discuss how to control nuclear spin generator system by using backstepping design. Firstly, an active backstepping design control method is presented for synchronizing two identical nuclear spin generator system with each other. It is a systematic design approach and consists of a recursive procedure interlacing the choice of Lyapunov function with the design of active control. Secondly, backstepping design is proposed for controlling uncertain nuclear spin generator system based on parameter identification. To achieve this an effective observer is designed to identify the unknown parameter of nuclear spin generator system and track any desired trajectory. Finally, numerical simulations are provided to show the effectiveness and feasibility of the developed designs.

IC/CTS4678/03: Lyapunov stability.

Organiser: Stanislaus Maier-Paape (RWTH Aachen, Germany)

Obstacle avoidance by artificial potential fields with asymptotic-stability properties. **Jito Vanualailai** (University of the South Pacific, Fiji), Shin-ichi Nakagiri (Kobe University, Japan), Bibhya Sharma (University of the South Pacific, Fiji) IC/CT3414/038

A recent application of the Direct Method of Lyapunov is one that deals with the geometric problems of finding a collision-free path for a moving solid object among other solid objects. This problem, which is called the "find path problem," is well-known in robotics and several ways of generating solutions have been proposed. Among the more theoretically elegant but computationally intensive algorithms are those that are based on some kind of graph search methods or geometric search algorithms. Basically, graph search methods seek to establish straight lines or connectivity graphs that allow obstacles to ŚseeŠ each otherŠs position, shape, and orientation.

Simpler algorithms tend to use physical analogies. In 1986, a potential field method was proposed by Khatib. In his approach, position-dependent artificial potential fields are placed around obstacles and collision-free can be generated by determining the number of repulsive and attractive poles. Many improvements to KhatibŠs method have been proposed since then. More recently, Tanner et al. (2003) proposed a novel artificial potential method based on inverse Lyapunov functions to control nonholonomic mobile manipulators.

It is also well-known however that the artificial potential methods have a major drawback, namely, the potential function may have local minima other than the goal configuration. This leads to the possibility of having a collision-free path leading not to the goal but to "traps" outside the target.

This paper proposes a point-mass obstacle avoidance system that is asymptotically stable, which means that the potential function - indeed, the Lyapunov function - of the system has no local minima other than the goal configuration in the pathwise-connected proper subset of free space which contains the goal configuration.

Reduction problems in multi-scale systems dynamics. **Lyudmila Kuzmina** (Kazan Aviation Institute, Russian Federation) IC/CT3943/038

The paper is devoted to the different aspects of mathematical modelling and qualitative analysis in dynamics of complex multi-scale systems, that are generated by applied problems of engineering practice. Main aims are the problems of optimal mechanical-mathematical modelling and the regular schemes of decomposition in engineering design. The generalization of the reduction principle, well-known in stability theory of A.M. Lyapunov, is important goal of engineering practice. A uniform methodology, based on Lyapunov's methods, in accordance with Chetayev's stability postulate, is developed. The presented approach, based on a combination of stability theory and perturbation theory methods, allows us to elaborate the general conception of the modelling, to work out the simple schemes of engineering level for decomposition-reduction of full systems and dynamic properties. This approach enables us to obtain simplified models that are of interest for applications, with rigorous substantiation of the acceptability. The conditions of qualitative equivalence between full and reduced models are determined, with extended estimations of N.G. Chetayev's type on infinite time interval. In the applications to multi-scale systems dynamics (for mechanical systems with gyroscopes, for electromechanical systems, for robotic systems,...) the obtained results enable us to construct the reduced models in a strict mathematical way. The interpretation of these formalized constructions (reduced models) leads to new approximate theories, acceptable in applications of engineering practice. It allows to optimize the analysis process and synthesis, to cut down the engineering design time. As applications various examples of concrete physical nature are considered.

Stability of perturbed dynamical systems. **Hammami Mohamed Ali** (University of Sfax, Tunisia) IC/CT825/003

We consider a time-varying nonlinear perturbed dynamical system. Under some growth sufficient conditions on the nominal system, we give a stability result of the system with perturbation. The exponential and uniform asymptotic stability are studied. A new Lyapunov function is also introduced to abtain a large class of stable systems.

A navigation and collision-avoidance scheme for heterogeneous robot collectives. **Bibhya Sharma** (University of the South Pacific, Fiji), Jito Vanualailai (University of the South Pacific, Fiji) IC/CT665/038

In this paper we propose a set of new continuous time-invariant acceleration controllers that considers the multi-task of control and motion planning of heterogeneous robot collectives within a dynamic but constrained environment. The dynamic obstacles will include members of the collective as well as other moving solids in the workspace. An dual avoidance scheme is introduced for a heterogenous 3-robot collective and the moving/static obstacles within a potential field framework. This, together with the other kinematic and the dynamics constraints have been treated simultaneously via a Lyapunov-based approach. We demonstrate the efficiency of the nonlinear algorithm with results through simulations of a couple of interesting situations.

Lyapunov's second method in problems of the stability of solutions of systems with impulse effect. **Alexander Ignatyev** (Donetsk, Ukraine) IC/CT4236/038

A system of ordinary differential equations with impulse effect at fixed moments of time is considered. The system is assumed to have the zero solution. It is shown that the existence of a corresponding Lyapunov function is a necessary and sufficient condition for the uniform asymptotic stability of the zero solution. Restrictions on perturbations of the right-hand sides of differential equations and impulse effects are obtained under which the uniform asymptotic stability of the zero solution of the 'unperturbed' system implies the uniform asymptotic stability of the zero solution of the 'perturbed' system.

Stability analysis of two-dimensional pool-boiling systems. **Stanislaus Maier-Paape** (RWTH Aachen, Germany) IC/CT4885/035

In this talk a model for pool-boiling systems is considered. This model involves only the temperature distribution within the heater and models the heat exchange with the boiling medium via a nonlinear boundary condition imposed on the fluid–heater interface. The model allows multiple homogeneous (i.e. spatially constant) and multiple heterogeneous steady-state solutions. The structure of this family of steady-state solutions has been studied by means of a bifurcation analysis in two recent papers by Speetjens, Reusken and Marquardt. The present study concentrates on stability properties of these steady-state solutions. To this end, a generic linear and a case-specific nonlinear stability analysis are performed which show that only the homogeneous steady-states of complete nucleate or complete film boiling are linearly stable. All heterogeneous steady-state solutions appear linearly unstable. These stability results are consistent with laboratory observations.

03: Nonlinear Analysis and Dynamical Systems, Posters

IC/PP852/030: **Control of the symmetric ball rolling without sliding or spinning.**

Presenter: Sebastián José Ferraro (Universidad Nacional del Sur, Argentina)
Co-author: Maria Etchechoury (Universidad Nacional de La Plata, Argentina)
Co-author: Hernan Cendra (Universidad Nacional del Sur, Argentina)

A ball having two of its three moments of inertia equal and whose center of mass coincides with its geometric center, is called a *symmetric ball*. The symmetric ball rolling without sliding or spinning on a horizontal floor is an interesting example of a nonholonomic system. The *dynamics* of this system has been thoroughly described in terms of Liouvillean functions (see *Rolling of a symmetric sphere on a horizontal plane without sliding or spinning*, Rep. Math. Phys. vol. 57, no. 3, 2006, and references therein). This is done using a geometric approach, the system is shown to be equivalent to a dynamical system on $S^2 \times S^1$. On the other hand, the *isoholonomic problem* for a massless ball rolling without sliding or spinning has been also recently studied, emphasizing the geometry of the problem (see *A nonholonomic approach to isoparallel problems and some applications*, Dyn. Syst. vol. 21, no. 4, 2006, and references therein). The so-called *plate-ball system* is one mechanism that allows to implement this kind of optimal control problem. In the present poster we perform a geometric study of the control of the symmetric ball, using results from the two previous references. In this case we use impulsive control. Numerical methods are also addressed.

IC/PP4797/030: **Multiple-delay feedback control.**

Presenter: Ulrich Parlitz (Universität Göttingen, Germany)
Co-author: Alexander Ahlborn (Universität Göttingen, Germany)

Multiple Delay Feedback Control (MDFC) with two, three or four different and independent delay times is used to stabilize steady states of various chaotic dynamical systems. A comparison with delayed feedback control methods that are based on a single (fundamental) delay time (Pyragas' TDAS, ETDAS) shows that MDFC is more effective for fixed point stabilization in terms of stability and flexibility, in particular for large delay times. This control method is also used for manipulating spatio-temporal chaos based on lumped local feedback with several different delay times. As illustrated with the two dimensional Ginzburg-Landau and the Fitzhugh-Nagumo equation MDFC can, for example, be used to suppress turbulent fluctuations, to convert chaotic spiral waves into guided plane waves and for trapping spiral waves.

IC/PP862/030: **Multiparametric frequency-domain criteria for stability of distributed systems with multiple equilibria.**

Presenter: Aleksey Perkin (Saint Petersburg State University of Architecture, Russian Federation)
Co-author: Vera Smirnova (Saint Petersburg State University of Architecture, Russian Federation)

We study the asymptotic behavior of distributed nonlinear control systems which can be described by integral Volterra equations of the type:

$$\sigma(t) = \sigma_0(t) - \int_0^t \gamma(t-\tau)\varphi(\sigma(\tau))\,\mathrm{d}\tau \qquad (t \geq 0)\,. \qquad (1)$$

Here the function $\sigma_0(t)$ describes the proper oscillations of the system and $\gamma(t)$ is its impulse transfer function. Two types of the system are considered. The first type includes the systems with a *stable* linear part; i.e., $\sigma_0(t), \gamma(t) \in L_1[0,+\infty) \bigcap L_2[0,+\infty)$ and with piecewise continuous nonlinear function φ which satisfies the sector condition $0 \leq \varphi(\sigma)\sigma \leq k\sigma^2$ $(k < +\infty)$. Systems of the second type have *critical* linear part; i.e., $\sigma_0(t) = \nu + \sigma_1(t)$, $\gamma(t) = \gamma_0 + \gamma_1(t)$ where ν, $\gamma_0 \in R$ and $\sigma_1(t)$, $\gamma_1(t) \in L_1[0,+\infty) \bigcap L_2[0,+\infty)$. Another feature of the second type is the periodicity of the nonlinear function. Systems of both types often have a non-unique equilibrium. Several new theorems are demonstrated which guarantee that every solution of the above equation tends to certain equilibrium as t tends to infinity. The theorems are proved by means of the method of *a priori* integral estimates, which is widespread in control theory[1].

The results are formulated in terms of the transfer function

$$\chi(p) = \int_0^\infty \gamma(t)e^{-pt}\,\mathrm{d}t \qquad \text{for } (p \in \mathbb{C})\,.$$

They have the form of frequency-domain inequalities. Thus, for systems of the first type (provided that certain restrictions on φ and χ are fulfilled) the following assertion is true. If there exist such non-negative values of parameters τ, ϑ, and ϱ the inequality

$$\Re\{(\tau + i\omega\vartheta + \varrho\omega^2)\chi(i\omega)\} > 0$$

holds for all $\omega \neq 0$, then any solution of the Volterra equation tends to an equilibrium as $t \to +\infty$.

New frequency-domain inequalities presented in the paper are generated with regard to additional differential properties of nonlinear functions. As a result, either the inequalities are supplied by additional varying parameters or the algebraic restrictions on varying parameters are weakened. Perfecting the frequency-domain criteria leads to improved estimates for boundaries of convergence domains in the space of system parameters.

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IC/PP4325/030: Mel'nikov–Samoilenko adiabatic stability problem.

Presenter: Yarema Prykarpatskyy (Akademia Górniczo-Hutnicza, Poland)

We develop a symplectic method for the investigation of invariant submanifolds of nonautonomous Hamiltonian systems and ergodic measures on them. The so-called Mel'nikov-Samoilenko problem for the case of adiabatically perturbed completely integrable oscillator-type Hamiltonian systems is studied on the basis of a new construction of "virtual" canonical transformations.

IC/PP3284/032: Mathematical and physical modelling of seismic faults.

Presenter: Alejandro Munoz-Diosdado (Insituto Politecnico Nacional, Mexico)

Modelling of seismic faults by using spring block systems on a frictional surface, requires to solve coupled differential equation systems with a great number of equations, in order to avoid this problem, the spring-block model is mapped into a continuous, non-conservative cellular automaton. In this work we analyse the models of Olami, Feder and Christensen (OFC) and Barriere and Turcotte (BT), those models can be used to mimic the dynamics of a seismic fault in two dimensions. We have in the OFC model two rigid plates that move relatively between them, the total force in each block is increased uniformly, until a site reaches a value limit and a relaxation process begins. The redistribution of the forces in the nearest-neighbor blocks, causes a chain reaction (synthetic earthquake). Every time the automaton is calculated a synthetic earthquake is obtained. We obtained catalogues of synthetic earthquake magnitude, which we can represent as a time series. Such series exhibit power law behavior so much for the magnitudes (Gutenberg-Richter law) as for the duration times. The analysis of these time series with methods of the non-linear dynamics provides interesting results; for example, the time series show multifractality for large values of the conservation level. We present variations of the original model to include the concept of asperity, they are regions on the seismic faults which can accumulate a great quantity of energy, when they broke they can give rise to earthquakes of great magnitude. The BT model is a fractal automaton model for modelling earthquakes; we study with this model foreshocks and aftershocks. Also in this model we obtain empirical relationships from real seismicity as the Gutenberg-Richter and the Aki law. Although these models are a great simplification for studying the dynamics of a real fault, they have properties that are related to real seismicity. They are interesting mathematical and physical applications to the study of earthquakes.

IC/PP4796/032: Cluster weighted modelling.

Presenter: Ulrich Parlitz (Universität Göttingen, Germany)
Co-author: David Engster (Universität Göttingen, Germany)

Cluster Weighted Modeling was first introduced by Gershenfeld et al. and combines density estimation of the input data with a functional relationship to the output data. This leads to a number of local clusters, each containing its own model for describing the observed data. The parameters are optimized using an Expectation-Maximization (EM) algorithm, leading to a local optimum in parameter space. Applications of Cluster Weighted Modelling to different forcasting and learning tasks are presented and evaluated, including modifications and extensions of the original algorithm.

IC/PP4960/028: Classical field theories with non-holonomic constraints.

Presenter: Joris Vankerschaver (Universiteit Ghent, Belgium)

Nonholonomic constraints in mechanics have a long and distinguished history, and have been the subject of renewed interest during the last decades. On this poster, we give an outline of the status of nonholonomic constraints in *classical field theories*: first of all, we establish a differential-geometric framework for such theories by extending some well-known methods from geometric mechanics. Secondly, we outline a physical example of a nonholonomic field theory. Finally we show how the underlying differential geometry may be exploited for the construction of geometric integration algorithms, and we discuss the accuracy of these methods.

IC/PP1077/036: A modelling approach to nutrient driven regime shifts in shallow coastal systems: competition between seagrass and macroalgae.

Presenter: Jose-Manuel Zaldivar Comenges (Joint Research Centre, Italy)

Pristine coastal shallow systems are considered as dominated by extensive meadows of seagrass species, which are assumed to take advantage of nutrient supply from sediment. An increasing nutrient input is thought to favour in a first phase phytoplankton and/or epiphytic micro-, macroalgae as well as opportunistic ephemeral macroalgae that coexist with seagrasses. The primary cause of shifts and succession in the macrophyte community are nutrients added to water, mainly nitrogen and phosphorus. A competition model between rooted seagrass and macroalgae has been developed to analyse the succession of primary producer communities in coastal lagoons and to analyse the characteristics of regime shift using bifurcation analysis. The model considers nutrient dynamics as well as shadowing effects.

IC/PP4945/038: Lyapunov stability of elliptic periodic solutions.

Presenter: Jifeng Chu Jifeng Chu (Tsinghua University, PR China)

Using the relation between the Hill's equations and the Ermakov–Pinney equations, we will given some interesting lower bounds of rotation numbers of Hill's equations. Based on the Birkhoff normal forms and the Moser twist theorem, we will prove that two classes of nonlinear, scalar, time-periodic, Newtonian equations will have twist periodic solutions, one class being regular and another class being singular.

IC/PP4874/038: Sufficient conditions for existence and approximate construction of forced periodic solutions in automatically controlled systems with hysteresis feedback.

Presenter: Michael Semenow (Russia)
Co-author: Anton Gulin (Novo Lipetsk, Russian Federation)
Co-author: Aleksandr Butov (Steklov Institute of the RAS, Russian Federation)
Co-author: Pasha Tolokonnikov (Tolokonnikov Pasha, Russian Federation)

Automatic controlled systems with the hysteresis feedback are studied in this paper. Dynamics of such systems is described by the set (system) of equations:

$$\dot{\mathbf{z}} = \mathbf{A}\mathbf{z} + \mathbf{b}u(t)\,, \tag{1}$$
$$u(t) = f(t, x(t), \xi(t))\,, \tag{2}$$
$$x(t) = (\mathbf{z}(t), \mathbf{c})\,, \tag{3}$$
$$\xi = l(\omega(t))\,, \tag{4}$$
$$\omega(t) = \Gamma[\omega_0]x(t)\,, \tag{5}$$

where $\mathbf{A}$ is a constant matrix with the dimension $n \times n$, $\mathbf{z}(t)$ - vector function with values in $\mathbb{R}^n$, $\mathbf{b}$, $\mathbf{c}$-fixed vectors from $\mathbb{R}^n$. Function $u = f(t, x, \xi)$ is supposed to be continuous on a population of variables and T-periodic one by the first argument. Equations (4)–(5) describes relations between entrance condition and result condition in some hysteresis converter.

The sufficient conditions of the existens and method of the approximate construction of the forced periodic solutions in system (1)–(5) are offered in this paper.

IC/PP1211/015: Robust analysis of discrete linear shift-invariant systems represented by an interval matrix.

Presenter: Juan Delgado-Romero (Instituto Tecnologico de Morelia, Mexico)

In this paper we describe a new bond in order to guaranteed the robust stability of a linear shift invariant system which is represented by an interval matrix. This bound is based in the bound of Juang. The uncerteinties are represented by an interval matrix. The system is represented in state variable with parametric uncertainty in the A matrix.

Let the interval matrix A, where $A = [L, U]$ and L and $U \in R^{n\times n}$, $A_0 = \frac{1}{2}(U - L)$ is the centroid matrix and $D = \frac{1}{2}(U - L)$ is the difference matrix, then the interval matrix is Schur stable if

$$\rho(A) \leq \rho(A_0) + \rho(\left|S\left(T_{re}^{-1}A_0T_{re}\right)\right|) + \left|T_{re}^{-1}\right| D\,|T_{re}| = \beta < 1$$

This paper is in collaboration with Prof. Rodolfo González-Garza.

IC/PP398/015: A chaotic–dynamic view of investment risk in emerging economies.

Presenter: Edgardo Jovero (Universidad Complutense de Madrid, Spain)

An open-economy neo-Keynesian model is developed which highlights market power and price-setting behavior as a source of the indeterminacy and structural instability characterizing the risk environment in emerging markets. This should explain why countries, which constitute the whole of the emerging economies as a group, provide different country investment risks individually.

This structural instability in the behavior of emerging countries can take the form of a Hopf bifurcation, the likelihood of which increases as the mark-up power increases. Evidence is presented as to the likelihood of a Hopf bifurcation occurring, using the qualitative geometric theory of nonlinear complex dynamical systems. The Keynesian view that structural instability globally exists in an emerging market economy is put forward, and therefore the need arises for policy to alleviate this instability in the form of dampened fluctuations is presented as an alternative view analyzing the nature of risk and its role in investment management.

MSC (2000) : 91B62 (mathematical economics), 37F45 (complex dynamical systems) PACS code: 89.67.Gh (economics, econophysics) JEL classification: F43 (economic growth of open economies) Keywords: risk, foreign capital, emerging markets, neo-Keynesian economics, Hopf bifurcation

04: Partial Differential Equations, Minisymposia

IC/MP93/004: Anisotropic curvature flow and its applications.

Organiser: Piotr Rybka (Uniwersytet Warszawski, Poland)
Co-organiser: Yoshikazu Giga (University of Tokyo, Japan)

In the theory of crystal growth the anisotropy plays an important role in the development of complicated patterns. In image processing several evolution equations are used to remove noise from images. Sometimes equations with anisotropic structure are more suitable for this purpose.

This minisymposium encompasses several topics related to partial differential equations (PDEs) whose structure is anisotropic. The derivation of models as well as mathematical and numerical analyses of the equations are within the scope of the session. There is a special emphasis on interface evolution equations with singular interfacial energy as well as total variation flow because they are related to each other. The feature of these equations is that the speed of evolution is determined by nonlocal quantities so, strictly speaking, it is not a PDE although it is considered as a limit of PDEs.

As a typical example we consider crystal growth from vapor or solution whose equilibrium shape has flat parts called facets. Another example is crystalline motion of surfaces which is less studied compared with motion of curves. As far as the crystal growth problem is concerned we are particularly interested in the problem whether or not a facet breaks during evolution. For a total variation flow which is very related to crystalline motion such a problem is also important. Because of the nonlocal nature of these problems the analysis of these equations is not conventional and several new ideas are necessary.

In this minisymposium we discuss these problems both from analytic and numerical point of view. Several analytic tools, including variational method, viscosity method and others are needed. Numerical approach includes a level set approach as well as other methods. However, we do not intend to exclude other kind of anisotropy which is useful to study crystal growth or image processing.

Anisotropic line tension for a step edge on an epitaxial surface. **Russel Caflisch** (University of California, Los Angeles, USA) IC/MT2073/004

This talk starts with an atomistic model for the dynamics of a step edge (or island boundary) on an epitaxial surface. A steady state solution is found through a kinetic balance rather than local equilibrium and is validated by comparison to KMC simulations. In the limit of large adatom diffusion rate, the resulting boundary condition at the step edge involves a line tension term that is consistent with the Gibbs-Thomson formula. This is an atomistic, kinetic derivation of the Gibbs-Thomson formula, in contrast to the usual derivation from a thermodynamic driving force.

Singular interfacial energy and faceting in epitaxial relaxation. **Dionisios Margetis** (Univ. Maryland at College Park, USA) IC/MT1028/004

At sufficiently low temperatures surfaces of crystalline materials have a continuum free energy density that is singular at high-symmetry surface orientations. This lack of smoothness originates from the existence of distinct line defects, "steps", on crystal surfaces. From the continuum standpoint, when crystal surfaces relax to become flat by surface diffusion, the energy density singularity gives rise to macroscopically flat surface regions, "facets". More generally, the use of an interfacial energy suggests a steepest-descent, “variational” treatment of facet motion.

In this talk I address the question: Is this “variational” approach the continuum limit of a physically reasonable, discrete step flow model? By adopting the view that facet edges are free boundaries I show that, in principle, the crystal microstructure affects macroscopic evolution through the motion of individual steps on top of facets. In particular, the collapse times of such steps enter the requisite boundary conditions for the continuum. I discuss the crucial role of step interactions by application of perturbation theory.

A new look on singular flows. **Piotr Mucha** (Uniwersytet Warszawski, Poland) IC/MT3953/004

The subject of our analysis is a parabolic system arising from the theory of singular curvature flows. Our model is a simplification of the original equation in the plane with an anisotropic energy density function whose Wulff shape is a square. Due to this fact the system becomes degenerated and singular. Our main goals are the well posedness and the precise qualitative analysis of the solutions we constructed. As a result we obtain a possible interpretation of the product of two Dirac’s deltas.

Presented results are a joint work with Piotr Rybka from Warsaw University.

A simple case of the driven singular mean curvature flow in the plane. **Piotr Rybka** (Uniwersytet Warszawski, Poland), Yoshikazu Giga (University of Tokyo, Japan) IC/MT1396/004

In many free boundary problems (FBPs) the interface evolves according to the Gibbs-Thomson law with kinetic undercooling. We have in mind growth of ice from vapor or growth of crystals from solution. Mathematically, the Gibbs-Thomson relation is a driven mean curvature flow for the interface. In the problems mentioned above the underlying surface energy density function γ is of poor regularity, hence we are lead to consider singular mean curvature. The driving term is the coupling to the diffusion field (e.g. supersaturation or temperature). However, in the present problem, we assume that it is given and enjoys some monotonicity property, which is valid in the full FBP.

We study the dynamics of the driven singular mean curvature flow in the plane if function γ is piecewise linear and its Wulff shape of a rectangle. We are mostly interested in the evolution of closed Lipschitz curves which are slight perturbations of rectangles. We show existence of solutions for a generic driving satisfying the mentioned above monotonicity property. However, our focus is the process of bending of initially flat facets.

The motivation for the present choice of the Wulff shape comes from the fact that a rectangle is a cross-section of a circular cylinder (which is an aproximation to a hexagonal prism being the equilibrium shape of ice) with a plane containing the symmetry axis.

IC/MP93/004: Anisotropic curvature flow and its applications. #2

Organiser: Piotr Rybka (Uniwersytet Warszawski, Poland)
Co-organiser: Yoshikazu Giga (University of Tokyo, Japan)

(For abstract, see session #1 above.)

Some diffusion equations with finite propagation speed. **José Mazón** (Universitat de València, Spain) IC/MT1954/004

To correct the infinite speed of propagation of the classical diffusion equation Ph. Rosenau proposed the tempered diffusion equation

$$u_t = \nu \operatorname{div}\Big(\frac{uDu}{\sqrt{u^2 + \frac{\nu^2}{c^2}|Du|^2}}\Big).$$

This equation was derived by Y. Brenier by means of Monge-Kantorovich's mass transport theory and he named it as the *relativistic heat equation*.

We prove existence and uniqueness of entropy solutions for the Cauchy problem for the quasi-linear parabolic equation $u_t = \operatorname{div}\mathbf{a}(u,Du)$, where $\mathbf{a}(z,\xi) = \nabla_\xi f(z,\xi)$ and f being a function with linear growth as $\|\xi\| \to \infty$, satisfying other additional assumptions. In particular, this class includes the relativistic heat equation and the some flux limited diffusion equation used in the theory of radiation hydrodynamics.

We also study the evolution of the support of entropy solutions of relativistic heat equation. We establish the following result.

Proposition *Let C be an open bounded set in $\mathbb{R}^N$. Let $u_0 \in (L^1(\mathbb{R}^N) \cap L^\infty(\mathbb{R}^N))^+$ with support equal to $\overline{C}$. Assume that given any closed set $F \subseteq C$, there is a constant $\alpha_F > 0$ such that $u_0 \geq \alpha_F$ in F. Then, if $u(t)$ is the entropy solution of the Cauchy problem for the relativistic heat equation with u_0 as initial datum, we have that:*

$$\operatorname{supp}(u(t)) = \overline{C} \oplus \overline{B_{ct}(0)} \quad \text{for all } t \geq 0.$$

Singular diffusivity and its applications. **Mi-Ho Giga** (University of Tokyo, Japan), Yoshikazu Giga (University of Tokyo, Japan) IC/MT2896/004

Equations with singular diffusivity is by now popular. Typical examples include crystalline flows in material sciences and total variation flows in image processing. It is also useful to calculate the graph of discontinuous viscosity solutions for evolution equations by a level set method, where the graph of solutions are regarded as evolving surfaces.

However, its analytic foundation has not yet well established. We consider a class of first order evolution equations whose solutions may develop jump discontinuities. We introduce a singular vertical diffusivity in our level set formulation and study whether or not its level set (which is expected to be the graph of solutions) is overturned. By formal analysis there is a threshold magnitude of singular diffusivity to prevent overturning if the magnitute is greater than the threshold value.

Anisotropic variational problems in imaging. **Martin Rumpf** (Universität Bonn, Germany) IC/MT3096/004

In this talk applications of anisotropic geometric evolution equations and anisotropic variational problems will be discussed. Thereby, sharp edges or corners can be explicitly encoded in PDE models in imaging. A local classification identifies certain anisotropies or singularities in 2D or 3D images. This classification is then encoded in suitable a anisotropic energy integrant and a gradient flow is applied to relax the resulting functional. The classification can be done *a priori* or in a joint approach directly incorporated in the variational approach. Particular applications are the extraction of rectangular cartoons pattern for aerial images of city regions, the restoration or 3D-MR-Angiography data, or the restoration of surfaces.

A variational formulation for a level-set representation of multiphase flow and area-preserving curvature flow. **Peter Smereka** (University of Michigan, Ann Arbor, USA) IC/MT5064/004

Variational descriptions for various multiphase level-set formulations involving curvature flow are discussed. A representation of n phases using $n-1$ level set functions is introduced having the advantage that constraints preventing overlaps or vacuum are not needed. The representation is then used in conjunction with our variational formulation to deduce a novel level set based algorithm for multiphase flow. In addition, a similar variational formulation is applied to area preserving curvature flow. In this flow, the area (or volume in 3D) enclosed by each level set is preserved. Each algorithm has been implemented numerically and the results of such computations are shown.

IC/MP97/015: Viscosity solutions of partial differential equations: recent advances and applications.

Organiser: Pierpaolo Soravia (Università degli Studi di Padova, Italy)
Co-organiser: Martino Bardi (Università degli Studi di Padova, Italy)

The theory of viscosity solutions provides the correct framework and a powerful toolbox for treating a number of 1st and 2nd order partial differential equations that are not in divergence form, especially Hamilton–Jacobi equations and quasi-linear or fully nonlinear degenerate elliptic or parabolic equations. Many applied problems can be studied with these methods, such as deterministic and stochastic optimal control and games, motion of interfaces, crystal growth, vision theory, Hamiltonian mechanics etc. [1,2,3,4,5]. The goal of this minisymposium is reporting some recent advances in the viscosity solutions theory and its applications. Main topics on which the minisymposium will focus are: front propagation with prescribed normal velocity, in particular problems with non-local terms, with singularities and discontinuities; homogenization of nonlinear PDEs with highly oscillating terms, including stochastic oscillations and singular perturbation problems for the dimension reduction of multiple scales systems.

[1] Crandall, M.G., Ishii, H. and Lions, P.-L.; User's guide to viscosity solutions of second order partial differential equations. Bull. Amer. Math. Soc. (N.S.) 27 (1992), pp.1–67.

[2] Bardi, M., Crandall, M. G., Evans, L. C., Soner, H. M. and Souganidis, P. E.; Viscosity solutions and applications. I. Capuzzo Dolcetta and P.L. Lions Eds., Lecture Notes in Mathematics, 1660. Springer-Verlag, Berlin; Centro Internazionale Matematico Estivo (C.I.M.E.), Florence, 1997.

[3] Bardi, M. and Capuzzo-Dolcetta, I.; Optimal control and viscosity solutions of Hamilton–Jacobi–Bellman equations, Birkhauser, Boston, 1997.

[4] Fleming, W.H. and Soner, H.M.; Controlled Markov processes and viscosity solutions, 2nd edition. Springer, 2006.

[5] Giga, Y.; Surface evolution equations – a level set method. Hokkaido University Series in Mathematics, 2002.

A level-set method for viscosity solutions with shocks. **Yoshikazu Giga** (University of Tokyo, Japan), Mi-Ho Giga (University of Tokyo, Japan) IC/MT2090/015

Solutions of first order equations or second order parabolic equations may develop jump discontinuities in finite time even if initial data is smooth. If the equation of first order is a conservation type like the Burgers equation, there is a notion of a weak solution called an entropy solution. A viscosity version describing a discontinuous solution was introduced several years ago. We note such a notion is applicable to some second order equations.

We further develop a level set method to describe motion of such discontinuous solution. For more practical purpose we introduce vertical singular diffusion term which prevents overturing of the graphs. This way is very convenient to calculate numerically by a level set method for the graph of discontinuous solutions.

The eqautions we studied has arised naturally from a crystal growth problem such as bunchings.

Recent results on dislocations dynamics and homogeneization. **Regis Monneau** (Ecole Nationale des Ponts et Chaussées, France) IC/MT1068/015

We will present two models describing the collective behaviour of dislocations defects in crystals. These models are mathematically written either as non-local Hamilton-Jacobi equations, or a coupled system of Hamilton-Jacobi equations. For these two systems, we will present homogenization results, describing at large scales the effective behaviour of densities of dislocations. As a by-product of our work, we will present rigorous results of homogeneization for a one-dimensional system of particules in interactions, as the number of particules goes to infinity.

Ergodic problem and periodic homogenization in half-space-type domains. **Francesca Da Lio** (Università degli Studi di Padova, Italy) IC/MT1833/015

We present some results related to the homogenization and ergodic problems for fully nonlinear elliptic boundary value problems in halph-space type domains with nonlinear Neumann boundary conditions. In particular we are interested in problems for which it is necessary to identify both the homogenized equation and boundary conditions.

Rates of convergence for the homogenization of fully-nonlinear second-order PDE in mixing random media. **Panagiotis Souganidis** (University of Texas at Austin, USA) IC/MT3798/015

I present new error estimates for the homogenization of second-order PDE in random mixing media with an algebraic rate. For linear equations the rate is algebraic while for fully nonlinear equations the rate is logarithmic.

IC/MP97/015: Viscosity solutions of partial differential equations: recent advances and applications. #2

Organiser: Pierpaolo Soravia (Università degli Studi di Padova, Italy)
Co-organiser: Martino Bardi (Università degli Studi di Padova, Italy)

(For abstract, see session #1 above.)

A new class of HJ equation with application to differential games. **Pierre Cardaliaguet** (Université Brest, France) IC/MT1460/015

In some two-player zero-sum differential games with asymetric information the value of the game—which depends on some parameter p in a convex way—turns out to be a viscosity subsolution of some HJ equation while its Fenchel conjugate w.r. to p is subsolution of a dual HJ equation. We show that these two conditions characterize the value. We also explain how approximate it and find explicit (Lax-Hopf) formulae.

Maximum principles for fully nonlinear elliptic and parabolic equations. **Andrzej Swiech** (Georgia Institute of Technology, USA) IC/MT2057/015

We will present various versions of generalized Alexandrov-Bakelman-Pucci (ABP) maximum principle for viscosity solutions of fully nonlinear elliptic and parabolic equations with superlinear-growth gradient terms and unbounded coefficients. The maximum principle may not hold for such equations however we will identify classes of equations for which some form of ABP maximum principle does hold. The results are obtained using the so called iterated comparison function method.

On the asymptotic behavior of solutions of p-Laplace equations as p goes to ∞. **Paola Loreti** (Universita' degli Studi di Roma "La Sapienza", Italy) IC/MT1163/015

Let $\Omega \subset \mathbb{R}^n$ be a bounded open set and $f \in C(\overline{\Omega})$. We consider, for $1 \ll p < \infty$ and $u \in W_0^{1,p}(\Omega)$, the following inhomogeneous p-Laplace equation:

$$\sum_{i=1}^{n} \frac{\partial}{\partial x_i}\Big(|Du(x)|^{p-2} \frac{\partial u(x)}{\partial x_i} \Big) = -f(x) \quad \text{in } \Omega .$$

with 0-Dirichlet boundary conditions; i.e.,

$$u(x) = 0 \quad \text{for } x \in \partial\Omega .$$

We consider the problem of the asymptotic behaviour of solutions as p goes to ∞.

The case where $n = 2$ and f is a positive constant corresponds asymptotically to a model having a torsional creep phenomenon for a prismatic elastoplastic rod.

The more general case $f > 0$ is studied in [1], and the limit of the sequence is the distance function from the boundary of Ω. Then, it is possible to generalize the result to the region ω where f vanishes, to non-negative functions f, by using an ∞-Laplace equation. Here we discuss some cases when f may change sign.

We also discuss about some properties of the maximizers for the functional $\int_\Omega f(x)v(x)\,dx$ in the space of functions $v \in C(\overline{\Omega}) \cap W^{1,\infty}(\Omega)$ satisfying $v|_{\partial\Omega} = 0$ and $\|Dv\|_{L^\infty(\Omega)} \le 1$, and about the connection between the above arguments.

The talk is based on a joint work with H. Ishii[2].

[1] Bhattacharya, T., DiBenedetto, E. and Manfredi, J.; Limits as $p \to \infty$ of $\Delta_p u_p = f$ and related extremal problems. Some topics in nonlinear PDEs (Turin, 1989). Rend. Sem. Mat. Univ. Politec. Torino 1989, Special Issue, pp.15–68 (1991).

[2] Hitoshi Ishii and Paola Loreti; Limits of solutions of p-Laplace equations as p goes to infinity and related variational problems. SIAM J. Math. Anal. 37 (2005), no.2, pp.411–43.

Viscous Hamilton–Jacobi equations. **Alessio Porretta** (Universita' di Roma Tor Vergata, Italy) IC/MT5069/015

IC/MP260/015: Applied mathematics in Latin America: part 1.

Organiser: Domingo Tarzia (CONICET - Univ. Austral, Rosario - ARGENTINA)
Co-organiser: Julio Claeyssen (Universidade Federal do Rio Grande do Sul, Brazil)

The goal of this minisimposium (Part 1) is to give an overview of the state of the art in diferent subjects related to partial differential equations, optimization and optimal control that are under current development in several regions of Latin America.

Numerical solution of a minimax ergodic optimal control. **María Soledad Aronna** (Universidad Nacional de Rosario, Argentina), Laura Aragone (Universidad Austral de Rosario, Argentina), Pablo Lotito (UNICEN de Buenos Aires, Argentina) IC/MT584/015

We consider an L^∞ minimax ergodic optimal control problem with cumulative cost. More precisely, we want to minimize the cost

$$J(x,\alpha) = \operatorname{ess\,sup}_{t\in[0,\infty)} \left\{ h(y(t),\alpha(t)) + \int_0^t g(y(\tau),\alpha(\tau))d\tau \right\}.$$

The control set are L^∞ function, h and g are data and the trajectory $y(\cdot)$ is given by an ordinary differential equation.
Obtaining the optimal cost function, defined by $u(x) = \inf_{\alpha\in\mathcal{A}} J(x,\alpha)$, is not easy in general. We approximate $u(x)$ as the supremum over $t > 0$ of the following evolution problems:

$$u(t,x) = \inf_{\alpha} \operatorname{ess\,sup}_{s\in[0,t)} \left\{ h(y(s),\alpha(s)) + \int_0^s g(y(\tau),\alpha(\tau))d\tau \right\}.$$

For these evolution problems we present the associated Hamilton-Jacobi-Bellman equation. As this HJB equation is consistent with a numerical procedure, we use this discretization to obtain a procedure for the primitive problem.
For the numerical solution of the ergodic version of this problem we will also need a perturbation of the instantaneous cost function. We give an appropriate selection of the discretization and penalization parameters to obtain discrete solutions that converge to the optimal cost.
We present numerical results made upon two examples.

On freezing of a finite humid porous medium with a heat-flux condition. **Eduardo Santillan Marcus** (Universidad Austral de Rosario, Argentina) IC/MT590/015

Let us consider the flow of heat and moisture through a finite porous half-space during freezing. The position of phase change front at time t, given by $x = s(t)$,divides the porous body into two regions. Let us denote by $u = u(x,t), v = v(x,t)$, and $w = w(x,t)$ the temperature distribution in the freezing region and the temperature distribution and the moisture distribution in the region where coupled heat and moisture flows respectively. In $0 < x < s(t)$ there is no moisture movement, and in $s(t) < x < 1$ the process of the coupled heat and moisture flows is described by the well known Luikov's system. Equivalence between this problem and a system of Volterra integral equations is found. The existence of a unique local solution in time for this problem is also obtained.

Littlewood–Paley spline wavelets: a simple and efficient tool for signal and image processing in industrial applications. **Eduardo Serrano** (Universidad Nacional de San Martín, Argentina), Maria Figliola (Fibertel, Argentina) IC/MT693/015

Wavelets play a significant role in applied mathematics when time-scale methods are required, or it performs better than Fourier methods. When the shift-invariance is needed or large scales phenomena are as important as small scales ones, the correct tool for analyzing is the Continuous Wavelet Transform.
This transform is not correlated with orthonormal wavelet bases or a multiresolution scheme. Otherwise, it gives us a continuous spectra of filtered versions of the signal resulting from its convolutions with the analyzing wavelet, well localized both in time and the frequency domain. However, a non trivial problem is to choice the analyzing wavelet, to compute the continuous transform from the sampled or experimental data and to deal with the numerical results.

Here we propose a simple option. We will call Littlewood–Paley wavelet, any one defined from the difference $\psi(t) = 2\varphi(2t) - \varphi(t)$, where $\varphi(t)$ is an appropriate basic function acting as low-pass filter. Then,the wavelet acts as a band-pass filter, having some null moments. We design the basic function in the cubic spline class. In this way, we get the numerical advantages of the spline framework. Simple and efficient algorithms can be developed.

Existence and multiplicity of solutions for elliptic problems arising in plasma physics with indefinite discontinuous nonlinearities. **Marco Calahorrano** (Escuela Politécnica Nacional, Ecuador) IC/MT786/015

In this paper we study the critical points for a locally Lipschitz functional that in some sense will be solutions of the elliptic problem with indefinite discontinuous nonlinearities. We should mention that our results were inspired by the work of Ambrosetti–Badiale, Arcoya–Calahorrano and Chang. For the problem studied in Ambrosetti,A., Badiale, M.(The dual variational principle and elliptic problems with discontinuous nonlinearities, *J. Math. Anal. Appl.*, **140** (1989), 363–373.), we introduce the indefinite nonlinearities as in Alama, S., Tarantello, G. (On semilinear elliptic equations with indefinite nonlinearities) and Berestycki, H., Capuzzo-Dolcetta, I., Nirenberg, L., (Variational methods for indefinite superlinear homogeneous elliptic problems, *NoDEA*, **2** (1995), 553–572) and we obtain the existence and multiplicity of solutions using the critical points theory developed by Chang in Variational methods for nondifferentiable functionals and their applications to partial differential equations, *J. Math. Anal. Appl.*, **80** (1981), 102–129.
Applications for Plasma Physics are considered with nonlinearities that change sign.

IC/MP260/015: Applied mathematics in Latin America: part 1. #2

Organiser: Domingo Tarzia (CONICET - Univ. Austral, Rosario - ARGENTINA)
Co-organiser: Julio Claeyssen (Universidade Federal do Rio Grande do Sul, Brazil)

(For abstract, see session #1 above.)

Well-posedness, stability and numerical results for the thermoelastic behavior of a coupled joint-beam PDE–ODE system modelling the transverse motions of the antennas of a space structure. **Ruben Spies** (IMAL (CONICET -UNL), Argentina), Eugene Cliff (Interdisciplinary Center for Applied Mathematics„ USA), Zhuangyi Liu (University of Minnesota, USA), Terry Herdman (Virginia Tech., USA) IC/MT798/015

A mathematical model for both axial and transverse motions of two beams with cylindrical cross-sections coupled through a joint is presented and analyzed. The motivation for this problem comes from the need to accurately model damping and joint dynamics for the next generation of inflatable/rigidizable space structures. Thermo-elastic damping is included in the two beams and the motions are coupled through a joint which includes an internal moment. Thermal response in each beam is modeled by two temperature fields. The first field describes the circumferentially averaged temperature along the beam, and is linked to the axial deformation of the beam. The second describes the circumferential variation and is coupled to transverse bending. The resulting equations of motion consist of four, second-order in time, partial differential equations, four, first-order in time, partial differential equations, four second order ordinary differential equations, and certain compatibility boundary conditions. The system is written as an abstract differential equation in an appropriate Hilbert space, consisting of function spaces describing the distributed beam deflections, and temperature fields, and a finite-dimensional space that projects important features at the joint boundary. Semigroup theory is used to prove the system is well-posed, and that with positive damping parameters the resulting semigroup is exponentially stable. Steady states are characterized and several numerical approximation results are presented.

Recent developments on the Boltzmann equation and its applications. **Liliane Barichello** (Universidade Federal do Rio Grande do Sul, Brazil) IC/MT656/015

In recent years, an increased interest in the general area of rarefied gas dynamics has been noted, essentially because of some applications related to micro-machines and microeletro-mechanical systems. However, research in this area is also related to aerospace applications and environmental problems, in particular, aerosol mechanics. This field is associated with the kinetic theory of gases as described by the integro-differential equation proposed by Boltzmann in 1872. A linear version of the Boltzmann equation is also a main tool in the treatment of radiative transfer problems (including bio-medical applications), neutron transport problems and the study of the behavior of electrons in semiconductors.

In this work we present recent results obtained from spectral methods, in deriving solutions for kinetic models of the Boltzmann equation. In particular, a wide class of solutions developed, for classical problems in the rarefied gas dynamics, by an analytical version of the discrete-ordinates method is discussed.

Eigenanalysis of multi-walled carbon nano-tubes by using the impulse response. **Julio Claeyssen** (Universidade Federal do Rio Grande do Sul, Brazil), Rosemaira Copetti (Universidade Federal de Santa Maria, Brazil), Teresa Tsukazan (Universidade Federal do Rio Grande do Sul, Brazil), Sandra Vielmo (Universidade Federal de Santa Maria, Brazil) IC/MT1492/015

We shall consider multi-walled carbon nanotubes (MWNT) modelled as an assemblage of Euler-Bernoulli or Timoshenko beams connected throughout their length by springs subject to van der Waals interaction between any two adjacent nanotubes. The intertube displacements modes correspond to noncoaxial intertube resonances. The beams are subject to arbitrary boundary conditions and damping. This later includes Kelvin-Voigt internal damping and external viscous damping. For determining frequencies and modes, we study a second-order evolution system on which the stiffness matrix depends upon the eigenvalue. For this we shall employ an approach in the physical domain that is based upon a fundamental matrix response. The basis generated by this response allows to simplify the boundary problem for determining the modes. This eigenanalysis will allow to study forced responses of MWNT under classical and non-classical boundary conditions. This approach can be useful in approximating real situations with sufficiently accuracy. The transient behavior of forced responses can be explicitly identified in terms of the impulse response.

Exact solution for a Stefan problem with convective boundary condition and density jump. **Domingo Tarzia** (CONICET - Univ. Austral, Rosario - ARGENTINA) IC/MT867/015

We consider the solidification of a semi-infinite material which is initially at its liquid phase at a uniform temperature T_i. Suddenly at time $t > 0$ the fixed face $x = 0$ is submitted to a convective cooling condition with a time-dependent heat transfer coefficient of the type $H(t) = ht^{-1/2}$ $(h > 0)$. The bulk temperature of the liquid at a large distance from the solid-liquid interface is T_∞, a constant temperature such that $T_\infty < T_f < T_i$ where T_f is the freezing temperature. We also consider the density jump between the two phases. We obtain that the corresponding phase-change (solidification) process has an explicit solution of a similarity type for the temperature of both phases and the solid-liquid interface, if and only if the coefficient h is large enough, that is $h > h_0 = \frac{k_l}{\sqrt{\pi \alpha_l}} \frac{T_i - T_f}{T_i - T_\infty}$ where k_l and α_l are the conductivity and diffusion coefficients of the initial liquid phase. Moreover, when $h \leq h_0$ we only have a heat conduction problem for the initial liquid phase and the corresponding change of phase does not occur.

IC/MP264/040: Recent advances in the analysis of nonlinear parabolic equations and their singular limits.

Organiser: Cyrill Muratov (New Jersey Institute of Technology, USA)
Co-organiser: Peter Gordon (New Jersey Institute of Technology, USA)

This minisymposium is devoted to recent advances in the analysis of reaction–diffusion and related problems which naturally arise in numerous applications such as combustion, phase transitions, and biological modeling. The focus of the talks will be on recent rigorous results on formation and global in time evolution of coherent structures. The first half of the talks will address problems of front propagation and failure in homogeneous and inhomogeneous media in the presence of advection. The second half will discuss a number of singular limits leading to the formation and non-trivial dynamics of topological defects, such as point defects, filaments and sharp reaction fronts. The analysis relies heavily on the tools of functional analysis, calculus of variations, maximum principle, and degree theory.

A variational approach to front propagation in infinite cylinders. **Cyrill Muratov** (New Jersey Institute of Technology, USA) IC/MT1071/040

In their classical 1937 paper, Kolmogorov, Petrovsky and Piskunov proved that for a particular class of reaction-diffusion equations on the line the solution of the initial value problem with the initial data in the form of a unit step propagates at long times with constant velocity equal to that of a certain special traveling wave solution. This type of a propagation result has since been established for a number of general classes of reaction-diffusion-advection problems in cylinders. In this talk I will show that actually in the problems without advection or in the presence of transverse advection by a potential flow these

results do not rely on the specifics of the problem. Instead, they are a consequence of the fact that the considered equation is a gradient flow in an exponentially weighted L^2-space generated by a certain functional, when the dynamics is considered in the reference frame moving with constant velocity along the cylinder axis. Independently of the details of the problem only three propagation scenarios are possible in the above context: no propagation, a "pulled" front, or a "pushed" front. The choice of the scenario is completely characterized via a minimization problem.

Boundary layers and KPP fronts in a cellular flow. **Alexei Novikov** (Penn State University, USA) IC/MT1074/040

The objective of this talk is to describe how fluid cellular flows with large intensity affect front propagation. We consider propagation of premixed flames with unit Lewis number in incompressible flows with asymptotically large intensity. The speed-up of flame-fronts and their structure will be determined. This work is done with L. Ryzhik.

Traveling waves in a 2D cylinder with undulating boundary and their homogenization limit. **Ken-Ichi Nakamura** (University of Electro-Communications, Japan) IC/MT2062/040

We discuss traveling waves for a curvature-driven motion of plane curves in a two-dimensional cylinder Ω with periodically undulating boundary. The law of motion of the curve is given by

$$V = \kappa + A,$$

where V denotes the normal velocity of the curve, κ denotes the curvature and A is a positive constant representing a constant driving force. This equation appears as a certain singular limit of an Allen-Cahn type nonlinear diffusion equation and the solution curve represents the interface between two different phases.

We study how the average speed of the periodic traveling wave depends on the geometry of the domain boundary $\partial\Omega$. More specifically, we consider the homogenization problem as the period of the boundary undulation, denoted by ε, tends to zero, and determine the homogenization limit of the average speed of periodic traveling waves. Quite surprisingly, this homogenized speed depends only on the maximum opening angle of the domain boundary and no other geometrical features are relevant. Our analysis also shows that, for any small $\varepsilon > 0$, the average speed of the traveling wave is smaller than A, the speed of the planar front. This implies that boundary undulation always lowers the speed of traveling waves, at least when the bumps are small enough.

This presentation is based on a joint work with Bendong Lou (Tongji University, China) and Hiroshi Matano (University of Tokyo, Japan).

Vortex and filament dynamics in Ginzburg–Landau theories. **Giandomenico Orlandi** (Università degli Studi di Verona, Italy) IC/MT1122/040

In a series of papers with F. Bethuel and D. Smets (Paris VI), we prove that, for the complex parabolic Ginzburg–Landau equation, asymptotically, vorticity evolves according to motion by mean curvature in Brakke's weak formulation. In the two dimensional case we prove that, in a suitable time scaling, vortices evolve according to a simple ordinary differential equation, which is a gradient flow of the Kirchhoff-Onsager functional. This convergence holds except for a finite number of times, corresponding to vortex collisions and splittings, which we describe carefully. The only assumption is a natural energy bound on the initial data.

IC/MP264/040: Recent advances in the analysis of nonlinear parabolic equations and their singular limits. #2

Organiser: Cyrill Muratov (New Jersey Institute of Technology, USA)
Co-organiser: Peter Gordon (New Jersey Institute of Technology, USA)

(For abstract, see session #1 above.)

A variational free-boundary problem arising in combustion theory. **Matteo Novaga** (Università di Pisa, Italy) IC/MT769/040

I will describe a variational approach applied to a singular limit of reaction–diffusion–advection equations which arise in combustion modeling. This approach allows to establish existence, uniqueness, monotonicity, asymptotic decay, and the associated free boundary problem for special traveling wave solutions which are minimizers of the considered variational problem. These minimizers are also demonstrated to be the limts of the minimizers of the corresponding approximating problems. I will also discuss matching upper and lower bounds for the speed of the minimizers in the singular limit, in terms of an area-type functional for small curvatures of the free boundary, leading to a rigorous justification of the Markstein model of flame motion.

On the κ–θ model of cellular flames: asymptotics and numerical simulations. **Claude-Michel Brauner** (Université de Bordeaux, France) IC/MT1620/040

Premixed gas combustion represents a rather intricate physical system involving fluid dynamics, multistep chemical kinetics, as well as molecular and radiative heat transfer. Its essential dynamical feature is formation of the so-called flame sheet propagating in a travelling wave type fashion. The basic propagation mode exhibits two main mechanisms of destabilization: one due to the thermal expansion of the gas known as the hydrodynamic instability, and the thermal-diffusive instability which is a result of the competition between the exothermic reaction and the heat diffusion. The thermal-diffusive instability manifests itself by generating a cellular structure, which in turn exhibits a chaotic dynamics. However, the cellular instability may be successfully captured by a simpler system comprised of only two equations. We consider the $\kappa - \theta$ model of flame front dynamics introduced by Frankel, Gordon and Sivashinsky. Its weakly nonlinear version reads:

$$\Phi_t + \frac{1}{2}\Phi_x^2 = \Phi_{xx} - \Theta, \tag{1}$$

$$\Theta_t + \Phi_x\Theta_x = \Theta_{xx} + \alpha\Phi_{xx} - \Theta. \tag{2}$$

Near the instability threshold ($\alpha = 1$), the front is arbitrarily close to the solution of the Kuramoto–Sivashinsky equation on a fixed time interval if the evolution starts from close configurations. We present numerical simulations that illustrate the theoretical results and also demonstrate the ability of the $\kappa - \theta$ to generate chaotic cellular dynamics.

This is joint work with M. Frankel, J. Hulshof, A. Lunardi, G.I. Sivashinsky and V. Roytburd.

Quenching, propagation and blow up in porous media combustion. **Peter Gordon** (New Jersey Institute of Technology, USA) IC/MT1073/040

Gaseous detonation is a phenomenon with very complicated dynamics which has been studied extensively by physicists, mathematicians and engineers for many years. Despite many efforts the problem is far from complete resolution. Recently Sivshinsky and his collaborators proposed the theory of subsonic detonation that occurs in hydraulically resistant porous media. This theory provides a model which is realistic, rich and suitable for a mathematical study. In particular, the model is capable of describing the transition from a slowly propagating deflagration wave to the fast detonation wave. This phenomena is known as a deflagration to detonation transition and is one of the most challenging issues in combustion theory. I will present some recent mathematical results concerning traveling front solutions arising in the context of the model. In particular, it will be shown that under very general assumptions the model admits traveling wave solutions. Moreover, these solutions unique in a presence of small but finite thermal diffusivity. This result strongly suggests that transition from deflagration to detonation is unavoidable unless quenching occurs. Some results on quenching, propagation limits of the combustion fronts and initiation of detonation in porous media will also be discussed. In particular, it will be shown that initiation of detonation can be formulated as a blow up problem.

Heat flows for director fields: the evolution of singularities. **Michiel Bertsch** (Consiglio Nazionale delle Ricerche, Italy) IC/MT1410/040

We discuss the evolution of director fields from domains in $\mathbb{R}^2$ or $\mathbb{R}^3$ to the unit sphere S^2. The simplest possible heat flow is described by the nonlinear parabolic system $u_t = \Delta u + |\nabla u|^2 u$, where the right hand side is generated by the Euler–Lagrange equation corresponding to the energy functional $\frac{1}{2}\int |\nabla u|^2 dx$. More complicated versions of this equation may contain additional terms which are important for the global dynamics of solutions, and they arise in the theories of liquid crystals or micromagnetism.

It is known that even in the case of smooth data classical solutions do not always exist globally; i.e., for all times. Singularities may occur in finite time, but it turns out that their evolution is not always uniquely determined by the data. In the talk we give an overview of recent results and present a list of open problems.

IC/MP149/040: Numerical verification methods for solutions of partial differential equations.

Organiser: Mitsuhiro Nakao (Kyushu University, Japan)
Co-organiser: Michael Plum (Universität Karlsruhe, Germany)

It is a purpose of this minisymposium to give a state of the art for the numerical approaches to the proof of the existence of solutions for partial differential equations(PDEs). Four speakers have been devoted for years to concerning research related to PDEs. Several kinds of leading principles of the verification methods will be presented by showing interesting and important numerial examples in applied analysis. These results would confirm us the actual effectiveness of the computer assisted proofs in the theory of nonlinear PDEs as well as suggest the methods to get useful *a posteriori* error estimates in mathematically rigorous sense for the numerical solutions of PDEs.

Computer assisted proofs for Navier–Stokes problems. **Mitsuhiro Nakao** (Kyushu University, Japan) IC/MT554/040

In this talk, we first give an overview of our numerical methods to verify, in mathematically rigorous sense, the existence of solutions for nonlinear elliptic boundary value problems. Our approach is based on the combination of fixed point theorems in functional spaces and the constructive error estimates of finite element (or spectral) method. Then, we describe on the way to apply the method to enclose the solution of the stationary Navier-Stokes equations with driven cavity flow in two dimension.

Our main topic in this talk consists of the clarlifying the global bifurcation structures in the heat convection problems known as Rayleigh-Bénard problem governing by the Navier-Stokes equation with nonlinear heat conduction. There are no longer any methods up to now in the existing theoretical approaches for such a complicated problems. Therefore, we considered a computer assisted approach to prove the existence of bifurcating solutions for the concerning problem.

First, under stress free boundary condistions on velocity, we derived several kinds of verified solutions for various Prandtl and Rayleigh numbers as well as to prove the existence of a symmetry breaking bifurcation point in two dimension. Second, we extend our results to three dimensional cases to be more difficult but more realistic and interesting bifurcation phenomena in the fluid mechanics. Overcoming various kind of difficulties of verification procedure compared with two dimensional case, several kinds of interesting solutions are verified, i.e., hexagonal, retangular, roll and mixed types, which will be shown in the presentation. Furthermore, we consider other boundary conditions by using different kind of base functions, e.g., Chebyshev series.

We believe that these methodologies and results should be actually significant and important from the viewpoint of the rigorous mathematical analysis on computer.

Numerical enclosures for photonic band gaps, I. **Michael Plum** (Universität Karlsruhe, Germany), Christian Wieners (Universität Karlsruhe (TH), Germany), Vu Hoang (Universität Karlsruhe (TH), Germany) IC/MT1017/040

We consider the propagation of optical waves in a periodic medium (*photonic crystal*), a problem which is mathematically described by the (homogeneous) Maxwell equations on the whole of $\mathbf{R}^n$, with periodic permittivity and permeability. The investigation of monochromatic waves leads to a spectral problem for the Maxwell operator. It is well known that the spectrum is characterized as a countable union of compact real intervals ("bands") $\Lambda_j = \{\lambda_j(\mathbf{k}) : \mathbf{k} \in \mathcal{B}\}$, with $\lambda_j(\mathbf{k})$ denoting the j-th eigenvalue of a Maxwell eigenvalue problem in the fundamental domain of periodicity, with quasi-periodic boundary conditions depending on a parameter $\mathbf{k}$ varying within the Brillouin zone $\mathcal{B}$, which is a known compact set in $\mathbf{R}^n$. Depending on the periodic material distribution, band gaps can occur, and in practical applications it is important to know (but analytically difficult to decide) if this really happens.

In this and the next talk by C. Wieners, we will attack this problem by computer-assisted means. In this talk, we present a method for reducing the task of computing $\lambda_j(\mathbf{k})$ for *all* $\mathbf{k} \in \mathcal{B}$ to *finitely many grid points* in $\mathcal{B}$. This is done by a perturbation argument based on *a priori* estimates for differences of Maxwell operators (with slightly different $\mathbf{k}$ values) and resolvent estimates, which result in enclosures for $\lambda_j(\mathbf{k})$ with $\mathbf{k}$ *between* the grid points in terms of enclosures for $\lambda_j(\mathbf{k})$ with $\mathbf{k}$ *in* the grid, which can be attacked numerically, as explained in the next talk by C. Wieners.

Numerical enclosures for photonic band gaps, II. **Christian Wieners** (Universität Karlsruhe (TH), Germany), Michael Plum (Universität Karlsruhe, Germany) IC/MT1016/040

As described in the previous talk by M. Plum, the problem of enclosing the spectral bands, and thus, of proving the occurrence of spectral gaps for photonic crystals (i.e., for Maxwell operators with periodic permittivity and permeability), can be reduced to enclosing the eigenvalues $\lambda_j(\mathbf{k})$ of the Maxwell operator on the fundamental domain of periodicity for *finitely many grid points* $\mathbf{k}$ in the Brillouin zone $\mathcal{B}$, and for finitely many j.
Here, we present a numerical method for the guaranteed enclosure of these eigenvalues. For this purpose, sufficiently close explicit eigenvalue bounds (based on techniques due to Weinstein, Kato, Rayleigh-Ritz, and Lehmann-Goerisch) are required. This has to be combined with a suitable sequence of comparison problems in order to provide additionally required information on the rest of the spectrum. Together with the perturbation method described in the previous talk, this numerical eigenvalue enclosure method can be used for rigorously proving the existence of band gaps for a given periodic material. Moreover, the method computes the band gap width within guaranteed bounds.

Finally, we present a numerical example for a 2-d periodic configuration, where we are able to prove the existence of a spectral gap; in this situation, no analytical approach to proving this is known. For this purpose, we use higher order finite element approximations, a Ritz-Galerkin eigenvalue solver, a parallel linear multigrid preconditioner, verified integration techniques, and interval arithmetic to control rounding errors.

A theorem for numerical verification of local uniqueness . **Nobito Yamamoto** (The University of Electro-Communications, Japan) IC/MT1415/040

Numerical verification methods, so called Nakao's methods, have been developed for computer-assisted proofs of existence of solutions to PDEs. The methods give guaranteed error bounds for calculated approximate solutions through error analysis of the approximation and fixed-point theorems.

PDEs are transformed into residual equations and transformed again into fixed-point equations. Then, for example, Schauder's fixed-point theorem is applied to prove the existence of the solutions. The conditions of the fixed-point theorem are modified through the error analysis and tried to verify using numerical techniques with computers.

In order to show the local uniqueness of the solution, we have applied a modified version of Banach's fixed-point theorem[1]. The version is intricately described in order to fit it to apply to Nakao's methods. In the present talk, we propose a generalized version of the previous work, which is simplified in the description from mathematical point of view and can be applied to more general problems.

The fixed-point equations are supposed to have Fréchet differentiable operators. Our theorem gives conditions in order that a given set of functions includes a unique solution to the fixed-point equation. Moreover, we show a lemma which concerns the mean value form for operators on function spaces which needs more additional conditions than the mean value form for functions on complex field. Numerical examples will be shown in order to explain how to apply our theorem.

[1] Yamamoto, N.; A numerical verification method for solutions of boundary value problems with local uniqueness by Banach's fixed point theorem. SIAM Journal on Numerical Analysis, Vol.35, No.5, (1998), pp.2004–2013.

IC/MP167/040: Dynamics of nonlinear waves in heterogeneous media.

Organiser: Yasumasa Nishiura (Hokkaido University, Japan)
Co-organiser: Jack Xin (University of California, Irvine, USA)

Nonlinear waves, such as kinks (fronts), pulses and spots, interact in various ways with inhomogeneous external environments. A representative case comes from the heterogeneity of the media that is generic in physics, chemistry, and biology. It may be a simple discontinuity, periodic or random media depending on the underlying phenomena. A wide variety of outputs have been observed after the interactions between those traveling waves and heterogeneous media such as penetration, repulsion, annihilation, splitting, propagation failures, and even more exotic behaviors including spatio-temporal chaos. At the same time many mathematical ideas have been extracted through the analysis of the above dynamics such as asymptotic averaging, effective properties, and reduction methods to ODEs. In this minisymposium, we bring together researchers who study these phenomena from numerical, analytical and experimental points of view, and show how they are interwoven in a unified way and make this field interesting. We also explore mathematical methods that are potentially applicable to a broad range of problems in this area.

Heterogenitiy-induced pulse dynamics in dissipative systems. **Yasumasa Nishiura** (Hokkaido University, Japan), Kei-Ichi Ueda (Kyoto University, Japan), Takashi Teramoto (Chitose Institute of Science and Technology, Japan) IC/MT2817/040

Particle-like (spatially localized) dissipative patterns arise in many fields such as chemical reaction, gas-discharge system, liquid crystal, binary convection, and morphogenesis. We discuss about the dynamics of moving particles in heterogeneous media, especially for the three types of heterogeneities: jump, bump, and periodic media respectively. Model systems include the Gray-Soctt model and a three-component reaction diffusion system of one-activator-two-inhibitor type. We focus on the following issues:(a) heterogeneity-induced defect-structure created around the jump point, (b) collision dynamics between particles and defects, (c) unstable objects called scattors which sort out the destinations of orbits, and (d) an organizing center creating traveling pulses, defects, and scattors via unfolding. When traveling objects like pulses or spots encounter heterogeneities, a variety of outputs are produced such as annihilation, rebound, splitting, and relaxing to an ordered pattern. It turns out that there is a class of unstable patterns called scattors which play a role of separator whose unstable manifolds guide the orbits to their destinations. For 1D case, a unified view is presented by a global solution branch with respect to the parameters chracterizing the heterogeneities that contain all the above important objects including traveling pulses, defects, and scattors.

Cell behaviors in heterogeneous media in an amoeba. **Toshiyuki Nakagaki** (Hokkaido University, Japan), Seiji Takagi (Hokkaido University, Japan), Ryo Kobayashi (Hiroshima University, Japan), Tero Atsushi (Hokkaido University, Japan), Tetsu Saigusa (Hokkaido University, Japan), Kei-Ichi Ueda (Kyoto University, Japan), Yasumasa Nishiura (Hokkaido University, Japan) IC/MT1810/040

The plasmodium of *Physarum polycephalum* in primitive creature of true slime mold is a large amoeboid organism, known as a good experimental model for studying physiology and dynamics of cell behaviors. Intracellular nonlinear waves and oscillations of biological activity have been reported in relation to cell behaviors and have been analyzed by nonlinear dynamics. In this talk, we will focus on effects of heterogeneous environment on cell behavior: indecisive behavior in crossing environmental barrier, and morphogenesis of cell shape under heterogeneous illumination of toxic light, etc. A simple mathematical

model for observed behavior is proposed in terms of dynamical system with a spatially heterogeneous parameter. Discussion is made on physiological significance of model dynamics.

Tango waves in inhomogeneous calcium excitable media. **Yuexian Li** (University of British Colombia, Canada) IC/MT3519/040

Oscillations and travelling waves are often observed in intracellular levels of calcium (Ca^{2+}) when egg cells are either activated by a sperm or by other kinds of stimuli. This is often due to the existence of Ca^{2+} stores that are capable of dynamically releasing Ca^{2+}, making the intracellular medium a Ca^{2+} excitable medium (Li et al, Am J Physiol 296:C1079, 1995). Tango waves are wave fronts that propagate in a back-and-forth manner and was found in a bidomain model of Ca^{2+} waves in frog eggs (Li, Physica D, 186:27, 2003). We show that such waves can occur in the presence of a time-dependent spatial inhomogeneity in an excitable medium. Analysis of such a phenomenon was carried out using the FitzHugh-Nagumo (FN) model with a spatially varying but time-independent term, $z(x)$, added to the first equation. Inhomogeneities cause pinning and oscillations of the front. This is best shown when $z(x)$ is a linear ramp. When the slope is large, it stabilizes the front. The front becomes less stable as the slope decreases. At a critical slope, the front becomes unstable through a Hopf bifurcation beyond which oscillations occur (Prat & Li, Physica D, 186:50, 2003). These results were generalized to a wider class of excitable media including systems of PDEs and IDEs (integral-differential equations) (Prat et al, Physica D, 202:177, 2005). In this talk, I will present a summary of these results.

Dynamics of localized patterns in heterogeneous media. **Kei-Ichi Ueda** (Kyoto University, Japan), Takashi Teramoto (Chitose Institute of Science and Technology, Japan), Xiaohui Yuan (Hokkaido University, PR China), Yasumasa Nishiura (Hokkaido University, Japan) IC/MT2050/040

We study pulse dynamics in one-dimensional heterogeneous media of bump type, namely one parameter of the system undergoes an abrupt change. Depending on the height of the bump, the responses of pulse behavior are penetration, rebound and splitting. Taking paramters close to singularities of codim 2 type consisting of drift and saddle-node instabilities, the PDE dynamics can be reduced to a finite-dimensional system which displays the three outputs. Moreover we show that steady solutions and their stable and unstable manifolds direct the flow of orbits.

IC/MP167/040: Dynamics of nonlinear waves in heterogeneous media. #2

Organiser: Yasumasa Nishiura (Hokkaido University, Japan)
Co-organiser: Jack Xin (University of California, Irvine, USA)

(For abstract, see session #1 above.)

Variational principles and reaction–diffusion front speeds in random flows. **Jack Xin** (University of California, Irvine, USA) IC/MT2779/040

An overview is presented on recent progress in analyzing reaction-diffusion front speeds in random flows with Gaussian statistics based on variational principles. Probabilistic tools such as path integral representations, properties of Gaussian processes (Borel inequality, growth law of running extrema), and large deviation methods are brought to action in concert with classical methods (comparison principle, multi-scale test functions). The front speeds depend on both the intensity and covariance of the random flows. Variational principle also allows efficient computation of speed statistics in lieu of direct simulations. Specific examples are front speeds in random shear flows, and randomly perturbed cell flows.

Homogenization for first- and second-order fully-nonlinear PDF in stationary ergodic media. **Panagiotis Souganidis** (University of Texas at Austin, USA) IC/MT3796/040

In this talk I will review recent developments in the theory of homogenization of fully nonlinear first- and second-order partial differential equations in random (stationary, ergodic) environments.

Speed-up of reaction-diffusion fronts by strong flows. **Andrej Zlatoš** (University of Chicago, USA) IC/MT2052/040

We present recent results on speed-up of traveling fronts by strong flows in reaction-diffusion equations. We characterize periodic flows which can arbitrarily speed up fronts for general combustion-type reactions in two dimensions, as well as those which achieve the fastest speed-up rates for KPP reactions in any dimension. Relations to quenching of reactions and to homogenization in the associated passive scalar equations will also be discussed.

Long-time dynamics to non-linear particle interacting systems of Maxwell type. **Irene Gamba** (University of Texas at Austin, USA) IC/MT3674/040

We study long time dynamics to solutions of initial value problems to a rather general multi-linear Boltzmann kinetic models of Maxwell type interactions that may describe qualitatively different processes in applications, but have many features in common. In particular we focus in the existence, uniqueness and asymptotics to dynamical scaling (self-similar) solutions and connections to Central Limit theorems for non-Gaussian states.

We use a relationship of spectral properties of the problem in Fourier space to study qualitative properties of the solution of the original initial value problem as well as the characterization of the domain of attraction to self-similar states. We clarify the connection with contractive measures for the pdf solution of the kinetic problem and discuss the optimal decay rates.

Examples are models of Maxwell type in classical space homogeneous, elastic or inelastic Boltzmann equation, and the elastic Boltzmann equation in the presence of a thermostat, all with finite or infinite initial energy, as well as Pareto distributions models in economy or more general Multiplicatively Interacting Stochastic Processes

This is in part a collaborative work with A. Bobylev and C. Cercignani.

IC/MP158/040: Nonlinear parabolic equations and their applications.

Organiser: Gieri Simonett (Vanderbilt University, USA)
Co-organiser: Patrick Guidotti (UC Irvine, USA)

This minisymposium features talks about theoretical aspects of nonlinear parabolic equations as well as their applications to Physics, Biology and Fluid Dynamics.

Global well-posedness for a model of haptotaxis. **Christoph Walker** (Vanderbilt University, USA), Glenn Webb (Vanderbilt University, USA) IC/MT1600/040

A system of non-linear partial differential equations modeling tumor invasion into surrounding healthy tissue is analyzed. The model incorporates haptotaxis, i.e., the directed migratory respond of tumor cells to the extracellular environment, as well as spatial and age structure of the tumor cells. Global existence and uniqueness of non-negative solutions is shown.

Asymptotic behaviour of some nonlocal problems. **Michel Chipot** (Universität Zürich, Switzerland) IC/MT1930/040

We investigate the asymptotic behaviour of nonlinear nonlocal equations and systems of parabolic type.

Large-time behavior of solutions of superlinear parabolic equations. **Peter Poláčik** (University of Minnesota, USA) IC/MT3399/040

We shall discuss several results on the large time behavior of solutions of nonlinear parabolic equations derived by means of parabolic Liouville theorems.

IC/MP158/040: Nonlinear parabolic equations and their applications. #2

Organiser: Gieri Simonett (Vanderbilt University, USA)
Co-organiser: Patrick Guidotti (UC Irvine, USA)

(For abstract, see session #1 above.)

Parabolic equations on singular manifolds. **Herbert Amann** (Universität Zürich, Switzerland) IC/MT1469/040

We will report on new results concerning the solvability of parabolic equations on manifolds with cusps, corners, and edges.

Maximal regularity for degenerate evolution equations with an exponential weight function. **Gieri Simonett** (Vanderbilt University, USA) IC/MT2957/040

In this talk we consider a class of degenerate evolution equations on the real line that have the distinguished feature that they contain an exponential weight function in front of the time derivative. Our interest is motivated by problems that arise from elliptic or parabolic equations on angles and wedges, and by free boundary problems with moving contact lines.

A modification of the Perona–Malik equation. **Patrick Guidotti** (UC Irvine, USA) IC/MT2532/040

A modification of the classical Perona–Malik equation of image processing is proposed which exhibits improved features at the analytical and at the practical level. The Perona–Malik is well-known to be ill-posed. The proposed modification has the advantage of being well-posed without introducing regularization terms which are known to lead to undesired blurring. The modification admits classical solutions and characteristic functions are stationary solutions; it also allows for a simple and effective discretization. Both analytical results and numerical experiments will be presented.

IC/MP50/015: Qualitative properties of nonlinear hyperbolic equations.

Organiser: Messaoudi Salim (King Fahd University, Saudi Arabia)
Co-organiser: Mokhtar Kirane (Université de La Rochelle, France)

We focus on qualitative studies of nonlinear hyperbolic equations and systems arising in various fields of applied sciences such as aeroelasticity, plasma physics, visoelasticity, geophysics and biology. Our aim is to bring together new ideas and methods for better understanding of many phenomena.

Our topics include: global existence, asymptotic behavior, finite time blow-up, transient profiles, and control.

Hyperbolic systems driven by controls taking values from the space of vector measures. **Nasiruddin Ahmed** (Université d'Ottawa, Canada) IC/MT691/0

Let I be a closed bounded interval, E, F separable Banach spaces and Σ the sigma algebra of subsets of the set I. The general system model considered in this paper is given by

$$dx = Axdt + B(dt)x + f(t,x)dt + g(t,x)\nu(dt), x = x_0, t \in I$$

where A is the infinitesimal generator of a C_0 semigroup on the Banach space E and B is an operator valued measure mapping Σ to $\mathcal{L}(E)$, the space of bounded linear operators on E, f is a nonlinear map from $I \times E$ to E and $g : I \times E \longrightarrow \mathcal{L}(F,E)$ and ν is any countably additive bounded F valued vector measure defined on Σ. We consider several control problems with objective (cost) functionals of the form

$$J(B) \equiv \int_I \ell(t,x)dt + \Psi(x(T)) + \varphi(\overline{B}) \longrightarrow \inf$$

where $\overline{B}$ denotes the total variation of the operator valued measure B. The infimum is taken over an admissible set $\mathcal{V}_{ad} \subset \mathcal{M}_{cabv}(\Sigma, \mathcal{L}(E))$, the space of countably additive bounded vector measures having bounded variations.

We present several results on existence of optimal policies under different assumptions and properties of the admissible set $\mathcal{V}_{ad}$. The abstract results are applied to structural control problems arising in theoretical mechanics, and hyperbolic and parabolic systems with coefficients containing measures.

Necessary conditions of optimality for such problems can be found in Ref 1.

(1): N.U.Ahmed, Differential Inclusions Operator Valued Measures and Optimal Control, Special Issue (Guest Editors, M.Michta, J.Motyl) Dynamic Systems and Applications, (2007).

Qualitative properties of a nonlilear wave equation. **Jorge Esquivel-Avila** (Universidad Autonoma Metropolitana, Mexico) IC/MT873/0

We consider a nonlinear wave equation without damping and with a superlinear source term. We analyze the qualitative behavior of solutions forwards and backwards for any value of initial energy. We present characterizations of blow-up, boundedness and convergence to the set of nonzero equilibria as $t \to \pm\infty$. In particular, we present the dynamics around the ground state in case that initial energy is equal to the mountain pass value. Usually, boundedness of global solutions is shown when the source term satisfies a condition on the superlineality. We avoid such restriction. We also consider initial energy bigger than the mountain pass value.

Solvability and regularity of a semi-linear hyperbolic equation with Neumann boundary control. **Andrzej Nowakowski** (University of Lodz, Poland) IC/MT795/0

The paper is devoted to study existence and stability of weak solutions for the following hyperbolic equations with controls in Neumann boundary conditions:

$$\begin{aligned} &x_{tt}(t,z) - \Delta_z x(t,z) = f(t,z,x(t,z)) \quad \text{a.e. on } (0,T)\times\Omega \\ &x(0,z) = \phi(0,z), \quad x_t(0,z) = \psi(0,z) \text{ on } \Omega \\ &\partial_\nu x(t,z) = v(t,z) \text{ on } (0,T)\times\Gamma, \quad v(t,z) \in \mathbf{V} \text{ on } (0,T)\times\Gamma, \end{aligned}$$

where Ω is a given bounded domain of $\mathbb{R}^n$ with boundary $\Gamma = \partial\Omega$ of C^2, $\Sigma = (0,T)\times\Gamma$, $\mathbf{V}$ is a given nonempty, closed set in R, $f : [0,T]\times\bar{\Omega}\times\mathbb{R} \to \mathbb{R}$, and $\varphi, \psi : \mathbb{R}^{n+1} \to \mathbb{R}$ are given functions, $\varphi(0,\cdot) \in H^1(\Omega)$, $\psi(0,\cdot) \in L^2(\Omega)$; $x : [0,T]\times\Omega \to \mathbb{R}$, $(x; x_t) \in C([0;T]; H^1(\Omega)) \times C([0;T]; L^2(\Omega))$ and $v : (0,T)\times\Gamma \to \mathbb{R}^m$ belongs to $L^2(\Sigma)$.

In I. Lasiecka and R. Triggiani, (Regularity theory of hyperbolic equations with nonhomogeneous Neumann boundary conditions. II. General boundary data, J. Differential Equations, 94 (1991), pp. 112–164), the existence and regularity problems for the above problem was study in a case of f independent on x with f belonging to $L^1(0,T;L^2(\Omega))$. We assume that the function f is nonlinear in x and under some specific assumption on it we prove that solution of our equation $(x; x_t) \in C([0;T]; H^1(\Omega)) \times C([0;T]; L^2(\Omega))$. Next under additional assumption if we take a sequence $L^2(\Sigma) \ni v_k \to v_0$ then we show that the corresponding sequence x_k of solutions of our problem is convergent in some defined sense to solution x_0 of our problem with v_0 on boundary.

About exponential stability to systems with indefinite damping. **Jaime Muñoz Rivera** (Laboratório Nacional de Computação Científica, Brazil) IC/MT2043/0

We consider system with indefinite damping and we prove under suitable hypotheses that the solutions decays exponentially to zero as time goes to infinity. We apply this results to the wave equation, viscoelastic system of memory type and to the Timoshenko's system for linear and non linear equations.

IC/MP50/015: Qualitative properties of nonlinear hyperbolic equations. #2

Organiser: Messaoudi Salim (King Fahd University, Saudi Arabia)
Co-organiser: Mokhtar Kirane (Université de La Rochelle, France)

(For abstract, see session #1 above.)

On existence, uniform decay rates and blow up for solutions of the 2D wave equation with exponential source. **Marcelo Moreira Cavalcanti** (Universidade Estadual de Maringá, Brazil) IC/MT4546/015

This work is concerned with the study of the nonlinear damped wave equation

$$u_{tt} - \Delta u + h(u_t) = g(u) \qquad \text{in } \Omega\times]0,\infty[,$$

where Ω is a bounded domain of $\mathbb{R}^2$ having a smooth boundary $\partial\Omega = \Gamma$.

Assuming that g is a function which admits *exponential growth at the infinity* and, in addition, that h is a monotonic continuous increasing function with polynomial growth at the infinity, we prove both: global existence as well as blow up of solutions in finite time, by taking the initial data inside the potential well. Moreover, optimal and uniform decay rates of the energy are proved for global solutions.

3D convective Cahn–Hilliard equation. **Varga Kalantarov** (Koc University, Turkey) IC/MT2208/0

We consider the initial boundary value problem for the 3D convective Cahn–Hilliard equation with periodic boundary conditions. This gives rise to a continuous dynamical system on $\dot{L}^2(\Omega)$. Absorbing balls in $\dot{L}^2(\Omega), \dot{H}^1_{per}(\Omega)$ and $\dot{H}^2_{per}(\Omega)$ are shown to exist. Combining with the compactness property of the solution semigroup we conclude the existence of the global attractor. We then proove the existence of an exponential attractor. This approach also gives an explicit upper estimate of the dimension of the exponential attractor, and of the global attractor.

Uniform stabilization of the wave equation on compact surfaces. **Valéria Neves Domingos Cavalcanti** (Universidade Estadual de Maringá, Brazil) IC/MT4547/015

This work is concerned with the study of the wave equation on compact surfaces and locally distributed damping, described by

$$u_{tt} - \Delta_M u + a(x)\, g(u_t) = 0 \quad \text{ on } M\times]0,\infty[,$$

where $M \subset R^3$ is an oriented embedded compact surface without boundary, such that $M = M_0 \cup M_1$, where

$$M_1 := \{x \in M; m(x)\cdot\nu(x) > 0\} \quad \text{and } M_0 = M\backslash M_1.$$

Here, $m(x) := x - x^0$, ($x^0 \in R^3$ fixed) and ν is the exterior unit normal vector field of M.

For $i = 1,\cdots,k$, assume that there exist open subsets $M_{0i} \subset M_0$ of M such that they are umbilical, or more generally, that the principal curvatures k_1 and k_2 satisfy $|k_1(x) - k_2(x)| < \varepsilon_i$ (ε_i considered small enough) for all $x \in M_{0i}$. Moreover suppose that the *mean curvature* H of each M_{0i} is *non-positive* (i.e. $H \le 0$ on M_{0i} for every $i = 1,\cdots,k$). If $a(x) \ge a_0 > 0$ on an open subset $M_* \subset M$ that contains $M\backslash\cup_{i=1}^k M_{0i}$ and if g is a monotonic increasing function such that $k|s| \le |g(s)| \le K|s|$ for all $|s| \ge 1$, then uniform decay rates of the energy hold.

On the long time behavior on some viscoelastic problems. **Said Berrimi** (King Fahd University, Saudi Arabia) IC/MT4079/0

In this minisymposium we will talk about the asymptotic behavior of the following initial boundary value problem:

$$\begin{cases} u_{tt} - \Delta u + \int_0^t g(t-\tau)\Delta u(\tau)d\tau + h(x,u_t) = f(u), & \text{for } x \in \Omega\,, t \geq 0 \\ u(x,t) = 0, & \text{for } x \in \partial\Omega\,, t \geq 0 \\ u(x,0) = u_0(x)\,, \quad u_t(x,0) = u_1(x)\,, & \text{for } x \in \Omega\,. \end{cases}$$

We study first the problem when: $h(x,u_t) = a(x)u_t\,|u_t|^m$ and $f(u) = -\,|u|^\gamma\,u$, for $m \geq 0$, $\gamma \geq 0$, and Ω is a bounded regular domain of $\mathbb{R}^n$ with $(n \geq 1)$, with regular boundary. We will prove an exponential decay result under weaker conditions on both a and g. In fact we will allow a to vanish on any part of Ω (including Ω itself). As a consequence, the geometry restriction imposed on a part of $\partial\Omega$ by Cavalcanti *et al.* in one of his recent papers, is dropped. Our method of proof is based on the use of the perturbed energy technique. Next we consider the problem when $h(x,u_t) = 0$ and $f(u) = |u|^\gamma\,u$, for $\gamma > 0$. We first prove a local existence theorem, then we show that, for certain initial data and suitable conditions on g and γ, that this solution is global with an energy which decays exponentially or polynomially depending on the rate of the decay of the relaxation function g.

IC/MP111/015: Singular differential equations in applied mathematics.

Organiser: Nikolay Sidorov (Irkutsk State University, Russian Federation)
Co-organiser: Vladilen Trenogin (Moscow State Institute of Steel and Alloys, Russian Federation)
Co-organiser: Boris Loginov (Ulyanovsk State University, Russian Federation)

This minisymposium concentrates on solutions of singular nonlinear operator equations especially applicable to algorithmic analysis of nonlinear DEs in mechanics and mathematical physics, and also to Volterra models of nonlinear dynamical systems in heat-and-power engineering. The authors expound recent results on local and global existence theorems, regularization, and identification, including asymptotic, numerical and group theoretic methods. The use of such methods in various problems in mathematics, modern physics, heat-and-power engineering, and mechanics (elasticity theory, phase transitions) has given the authors rich possibilities for creativity and applications. We also intend to explore these methods to nonlinear models of manufacturing polymer and improve communication between scientists active in this field.

Subgroup structure of branching equations with crystallographic group symmetries. **Oleg Makeev** (Ulyanovsk State University, Russian Federation), Boris Loginov (Ulyanovsk State University, Russian Federation) IC/MT190/015

In branching theory of solutions of nonlinear equations symmetry breaking problems are known, when at the passage of bifurcational parameter its critical value, solutions with crystallographic groups symmetry arise. Symmetries of simple cubic lattice and planar crystallographic groups in stationary and dynamic branching with applications to mathematical physics problems (phase transitions in statistical theory of crystal; capillary-gravity surface waves) were considered in works of the authors [1, 2] and bibliography to them. Special attention in these works was payed to subgroup structure of bifurcating solutions with respect to point subgroup of simple cubic lattice and in particular relatively normal divisors of this subgroup.

Here for stationary and Andronov-Hopf bifurcations with symmetry of the highest crystallic classes of basic syngonies (crystallic systems) of crystallographic groups as semi-direct products of translations on the basic directions and point symmetry of lattices subgroup structure of relevant branching equations and bifurcating solutions dual to subgroup structure of such symmetries is investigated. Applications to phase transition theory in physics are given.

1. B.V. Loginov, The solutions branching of nonlinear equations and group symmetry. Vestnik of Samara State Univrsity, 1998, N 2(8), 15-70

2. Makeev O., Loginov B., Computer realization of the branching equation construction on allowed group symmetry. Wang Y., Hutter K. - eds. Trends in applications of mathematics to mechanics. Proceedings of the international symposium, STAMM, Seeheim, Germany, August 22-28, 2004. Aachen: Shaker. Berichte aus der Mathematik, 277–288 (2005).

Variational splines for numerical solution of singular differential equations. **Igor Lutoshkin** (Ulyanovsk State University, Russian Federation), Vladimir Gorbunov (Ulyanovsk State University, Russian Federation), Name Martinenko (Ulyanovsk State University, Russian Federation) IC/MT752/0

The problem to be solved numerically is the initial one for an implicit ODE $F(\dot{x},x) = 0$, for $0 \leq t \leq T$ with $x(0) = x^0$, where $x \in \mathbb{R}^n$ and $F : \mathbb{R}^{2n} \to \mathbb{R}^n$ is a smooth transformation, in the case of arbitrary degeneracy of the Jacobi matrix $\partial F(\dot{x}(t),x(t))/\partial\dot{x}$ on the solution $x(t)$.

The proposed numerical method is based on the minimization of discrepancy of appropriate differential system and approximation of solution $x(t)$ by splines with moving knots. The first and second derivatives of the discrepancy functional on the spline's parameters can be effectively calculated with help of variational techniques and adjoint variables[1,2]. Here we present also a simpler techniques for direct differentiation of the discrepancy with respect to the parameters[3]. Comparative analytical and numerical analysis of different variants of the PM will be presented.

[1] Gorbunov, V.K. and Lutoshkin, I.V.; Development and experience of applying the parameterization method in degenerate problems of dynamical optimization. In Izv. RAN: Teor. Syst.,Upravl. 2004. No.5, pp.67–84.

[2] Gorbunov, V.K. and Lutoshkin, I.V.; The parameterization method in optimal control problems and differential-algebraic equations. In J. Comput. Appl. Math. (Elsevier) Vol.185, (2006) pp.377–390.

[3] Gorbunov, V.K. Lutoshkin, I.V. and Martynenko, Yu.V.; The parameterization method for singular differential equations. In Trudy Srednevoljskogo Matematicheskogo Obschestva (in Russian). Vol.8. (2006) pp.36–50.

IC/MP111/015: Singular differential equations in applied mathematics. #2

Organiser: Nikolay Sidorov (Irkutsk State University, Russian Federation)
Co-organiser: Vladilen Trenogin (Moscow State Institute of Steel and Alloys, Russian Federation)
Co-organiser: Boris Loginov (Ulyanovsk State University, Russian Federation)

(For abstract, see session #1 above.)

Analytical case of Lyapunov theorem about stability on first approximation. **Vladilen Trenogin** (Moscow State Institute of Steel and Alloys, Russian Federation) IC/MT135/015

Let X be real and complex Banach space. We consider the following differential equation:

$$\dot{x} = Ax + R(t,x). \quad (1)$$

Let here and below the following conditions are fulfilled
I. Let A be closed linear operator, mapping dense domain $D(A)$ in X and be generating operator of semigroup $U(t) = \exp(A(t)$ of class C_0. Semigroup U(t) is exponentially decreasing, i.e. there are constants $M > 0$ and $\alpha > 0$ such as for all $t \in \Re^+ = [0, +\infty)$ the following condition $||U(t)|| \le M\exp(-\alpha t)$ is fulfilled.
II. Nonlinear operator $R(t,x)$ is defined and continues wrt $t \in \Re^+$ and is analytical operator wrt x in point $x = 0$, $R(t,x) = \sum_{k=2}^{+\infty} R_k((t)x^k$, where $R_k(t)$ is k-linear bounded operators in X, and majourant numeric series has nonzero radius of convergence. Let call the classic solution of differential equation (1) on semi-axis $[0,\infty)$ the function $x = x(t)$ such that on $\Re^+$ this function is differentiable $x(t) \in D(A)$, and this function is solution of (1) on $\Re^+$. From condition II follows that DE (1) has trivial classic solution $x(t) = 0$. Apart from DE (1) we consider its first approximation the linear DE

$$\dot{x} = Ax. \quad (2)$$

For (1) and (2) we set the Couchy problem: to find their classic solutions, satisfies initial condition

$$x(0) = x_0. \quad (3)$$

If $R(t,x)$ do not depends on t, then DE (1) can be addressed as abstract dynamic system, its solutions as trajectories in phase space X, and point $x = 0$ - as equilibrium position of DE(1). We found the conditions when Lyapunov theorem about asymptotic stability of the classic trivial solution of DE (1) on its first approximation (2) is fulfilled.

For beginning we study the generalized solutions of Couchy problem (1),(3), i.e. continues solutions of integral equation

$$x(t) = U(t)x_0 + \int_0^t U(t-s)R(s,x(s))ds. \quad (4)$$

Definition. Let $\gamma > 0$. Space C_γ we call set of all abstract functions $x(t)$, defined and continues on semi-axis $\Re^+$ with operations of summation and multiplication on scalars and with results in X, for which the norm $|||x|||_\gamma = sup_{\Re^+}||x(t)||exp(\gamma t)$. The existence and uniqueness of generalized solution in space C_γ are proofed. This solution is analytic wrt x. For Ghelder operator $R_k(t)$ its proofed that generalized solutions is classical. We address the applications of this theory in problems for functional-differential equations and reaction-diffusion systems.

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2. V. A. Trenogin. *Functional Analysis.* Fizmatlit. Moscow, 2002 (Nuaka -1980, 1993)
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4. V. A. Trenogin. *First Lyapunov method for the abstract parabilic equations.* Abstracts of ISAAC-2005, pp. 15–16, Univ. of Catania.
5. V. A. Trenogin. *Abstract Dynamic Systems and First Lyapunov Method.* Proceedings of the S.M.Nikolsky 100 Anniversary. Moscow, RAS, 2005, p. 225
6. V. A. Trenogin. *Lyapunov Theorem on Stability wrt Linear Approximation as Corollary of the Implicit Function Theorem.* Doklady RAN, 2006, vol. 407, N 6, p. 7432-7436.

The theory of fundamental operator-functions of singular differential and integral operators in Banach spaces. **Michail Falaleev** (Irkutsk State University, Russian Federation) IC/MT232/015

We present principal results of the theory of fundamental operator-functions of singular differential and integral operators in Banach spaces. In explication of all theorems have employed the apparatus of generalized Jordan chains, the theory of generalized functions in Banach spaces, methods of semigroups with kernels. Such a mixture of diverse methods has given the possibility of investigating a wide class of singular differential and integral operator equations and partial differential operator equations with the Noether operator in the main part. In a number of classes of singular differential operator equations has been completely investigated.

1. N.Sidorov, B.Loginov, A.Sinitsyn, and M. Falaleev. *Lyapunov-Schmidt Methods in Nonlinear Analysis and Applications,* Dordrecht: Kluwer, 2002.

2. M.V.Falaleev and E.Yu. Grazhdantseva*Fundamental Operator Functions of Singular Differential Operators under Spectral Boundedness Conditions,* in Differ. Uravn. 2006. V. 42. No 6. P.769-774.

3. M.V. Falaleev. *Fundamental Operator Functions of Singular Differential Operators in Banach Spaces,* in Sibirsk. Mat. Zh., 2000. V.41. No 5. P.1167-1182.

Generalized solutions of integral-functional equations: construction and applications in power industry. **Nikolay Sidorov** (Irkutsk State University, Russian Federation), Denis Sidorov (Irkutsk, Russian Federation), Andrey Trufanov (Irkutsk State University, Russian Federation) IC/MT112/015

The method of construction of the generalized solutions with point carrier in singular part is proposed for nonlinear Volterra integral-functional equations

$$\int_0^t K(t,s)(x(s) + ax(\alpha s) + g(s^l x(s), s))\mathrm{d}s = f(t)$$

with sufficiently smooth kernel and function f; α and a are constants, and $0 < |\alpha| < 1$. The solution is constructed as a sum of singular and regular components. The special system of linear algebraic equations is used for construction of the singular component. The regular part is constructed by method of successive approximations combined with method of undetermined coefficients. The theorems of existence and uniqueness of the generalized solutions are proved. In general case the equation has a few bifurcating solutions. Such solutions can be constructed based on the results of this work in combination with known methods of bifurcation theory. Our results can be generalized on the systems and integral-operator equations, where kernel K is linear, and g is nonlinear mapping in Banach space. These results can be used in development of theory and application of differential-operator equations with Fredholm operator in main part[1] in problems of nonlinear dynamics and identification[2], and in other problems formulated in terms of the Volterra integral equations of the first kind.

[1] N. Sidorov, B. Loginov, A. Sinitsyn, M. Falaleev; Lyapunov–Schmidt Methods in Nonlinear Analysis and Applications. Kluwer Academic Publishers, Dordrecht, 2002.
[2] S. T. Zavalishin, A. N. .Sesekin; Dynamic Impulse Systems: Theory and Applications. Kluwer Academic Publ., Dordrecht, 1997.
[3] D. N. Sidorov; Modeling of Noninear Nonstationary Dynamic Systems by the Volterra Series: Identification and Applications. Siberian Journal of Industrial Mathematics. 2000, Vol. 3, No. 1(5), pp.182–195.

Andronov–Hopf bifurcation and group symmetry for differential equations non-resolved under derivative. **Boris Loginov** (Ulyanovsk State University, Russian Federation), Oleg Makeev (Ulyanovsk State University, Russian Federation), Irina Konopleva (Ulyanovsk State University, Russian Federation), Youri Rousak (Ulyanovsk State University, Russian Federation) IC/MT175/015

In previous our articles [1, 2] in Banach spaces E_1, E_2 the general problem of branching theory $F(x,\varepsilon)=0$, $F(x_0,0)=0$ with Fredholm operator $B_{x_0}=-F'(x_0,0)$ under group symmetry conditions $\mathcal{K}_g F(x,\varepsilon)=F(L_g x,\varepsilon)$ ($g\in G$ is a Lie group) was studied in the assumptions about potentiality or pseudopotentiality of the relevant branching equation (BEq). On the base of the general theorem on the group symmetry inheritance by BEq the cosymmetric identity for BEq with Lie algebra operators and the theorem on the BEq reduction (dimension lowering) in the case of non-invariant kernel were proved. Applications to bifurcation symmetry breaking problems were given.

In this communication Andronov–Hopf bifurcation for the differential equations non-resolved under derivative $F(p,x,\varepsilon)=0$, $p=\frac{dx}{dt}$, $F(0,x_0,\varepsilon)\equiv 0$ with Fredholm operators $A_{x_0}=F'_p(0,x_0,0)$, $B_{x_0}=-F_{x_0}(0,x_0,0)$ under Lie group symmetry is investigated by the same methods under potentiality or pseudopotentiality of the relevant branching equation. The analogous BEq reduction theorem is proved.

1. B.V. Loginov, I.V. Konopleva, Yu.B. Rousak, Symmetry and potentiality in general problem of branching theory, Izvestiya VUZ, Mathematics, 2006, N 4, 30-40.

2. B.V. Loginov, I.V. Konopleva, Yu.B. Rousak, Nonlinear operators with symmetry and potential branching equations. Proc. of Int. Conf. CAIM-XI, May 29-31, 2003 (A. Georgescu – ed), Oradea University, Romania 2003, v.1, 153–158

IC/MP2055/042: Quantum kinetic theory for Bose–Einstein condensation.

Organiser: Weizhu Bao (National University of Singapore)
Co-organiser: Hailiang Li (Capital Normal University, PR China)

The experimental realization of Bose–Einstein condensates (BEC) in magnetically trapped atomic gases at ultra-low temperature has spurred great excitement in the atomic physics community and renewed the interest in studying the macroscopic quantum behavior of the atoms. Theoretical predictions of the properties of BEC like the density profile, collective excitations and the formation of quantized vortices can now be compared with experimental data. This dramatic progress on the experimental front has stimulated a wave of activity on both the theoretical and the numerical front. In this minisymposium, the speakers will address recent advancements in the following directions:

(a) Mathematical analysis for quantum Boltzmann equation for BEC at finite temperature;
(b) Efficient and accurate numerical methods for quantum Boltzmann master equation;
(c) Analysis and simulation for the Gross–Pitaevskii equation.

Nonlinear fluid-dynamic PDEs and multiscale analysis. **Shu Wang** (Beijing University of Technology, PR China) IC/MT1378/025

In this talk asymptotic limits and multiscale-analysis problems of some macroscopic fluid-dynamic partial differential equations are studied. These asymptotic limits conclude quasineutral limit and nonrelativistic limit etc. while the nonlinear Fluiddynamic PDEs concern some models like Euler-Maxwell system, e-MHD system, Euler-Poisson system, Navier-Stokes-Poisson system and Drift-Diffusion system etc, widely used in the area of applied sciences such as semiconductors, plasmas, fluid dynamics and so on, and they are full of multiscale phenomena. Some formal and rigorous convergence results are given and some new methods or ideas are reviewed.

Kinetic numerical methods for ideal quantum gas dynamics. **Joe Yang** (National Taiwan University) IC/MT538/025

Numerical methods for solving the ideal quantum gas dynamics based on the Bose–Einstein and Fermi–Dirac distributions are presented. Both concepts of beam scheme and kinetic flux splitting scheme are extended and generalized to the convectional quantum Boltzmann equation. Formulations for one to three spatial dimensions are derived. Numerical experiments to validate the methods are first demonstrated on one-dimensional problems. Higher-order methods based on modern high-resolution non-oscillatory interpolation are implemented for practical calculations. The possible extension to higher-order transport is outlined and some potential applications are also given.

MS number: IC/MP/025/R/226 Mathematical Analysis and Numerical Simulation for Bose-Einstein Condensation

Numerical methods and kinetic modelling of Bose–Einstein condensation. **Lorenzo Pareschi** (Università degli Studi di Ferrara, Italy) IC/MT2300/025

We develop efficient numerical schemes for the quantum Boltzmann equation that preserve the main physical features of the continuous problem, namely conservation of mass and energy, the entropy inequality and generalized Bose-Einstein distributions as steady states. These properties are essential in order to develop numerical methods that are able to capture the challenging phenomenon of bosons condensation. We also show that the resulting schemes can be evaluated with the use of fast algorithms. In order to study the evolution of the condensate wave function the Gross-Pitaevskii equation is presented together with some schemes for its efficient numerical solution and the possibility of coupling this equation with the quantum Boltzmann equation is discussed.

Fokker–Planck–Boltzmann near Maxwellian. **Hailiang Li** (Capital Normal University, PR China) IC/MT1633/025

We consider the Fokker–Planck–Boltzmann equation viewed as the Boltzmann equation with additional diffusion term in velocity space to describe for instance the transportation in thermal bath of binary elastic collisional particles. The strong solution for initial data near an absolute Maxwellian is proven to exist globally in time. The effect of the diffusion in phase space is investigated. It produces a diffusion process in velocity space and results in a heating process on the macroscopic fluid-dynamical observable, and accelerates the convergence of solutions to the equilibrium of self-similar Maxwellian at the faster time-decay rate than Boltzmann equation. Moreover, the Fokker–Planck–Boltzmann equation is shown to converge under an appropriate scaling strongly to the Boltzmann equation in the process of zero diffusion limit.

IC/MP2055/042: Quantum kinetic theory for Bose–Einstein condensation. #2

Organiser: Weizhu Bao (National University of Singapore)
Co-organiser: Hailiang Li (Capital Normal University, PR China)

(For abstract, see session #1 above.)

Bloch-decomposition-based pseudospectral methods for quantum dynamics with periodic potentials. **Shi Jin** (University of Wisconsin, Madison, USA) IC/MT1343/025

We present a new numerical method for accurate computations of solutions to (linear) one dimensional Schrödinger equations with periodic potentials. Our approach is based on the classical Bloch decomposition method and it proves to be superior to the mainly used time-splitting spectral schemes. Indeed it is is shown by the given numerical examples, that ou r method is unconditionally stable, highly efficient and allows for much larger time-steps than the the splitting schemes.

Strong confinement for the Gross-Pitaevski equation: energy solutions. **Naoufel Ben Abdallah** (Université Paul Sabatier Toulouse III, France) IC/MT4487/042

The limit of the Gross-Pitaevskii equation with a partial strong confinement is considered. The obtained system is an infinite system of coupled Schrödinger equations in the non strongly confined direction. In a previous work (see the talk of F. Méhats), strong local solutions are constructed for the limit system and convergence is proven. The aim of this talk is to construct global energy solutions for the limiting system. The proof is based on a an averaged Gagliardo Nirenberg inequality. Convergence issues will also be adressed. This is a work in collaboration with F. Castella and F. Méhats.

Semi-classical analysis for the nonlinear Schrödinger equation with potential. **Rémi Carles** (Universität Wien, Austria) IC/MT513/025

We present some results concerning the semi-classical limit of the nonlinear Schrödinger equation with a potential, in two cases:

- Weak nonlinearity, when the potential is an harmonic potential. This study includes the description of the solution beyond caustics.
- Strong nonlinearity and general sub-quadratic potential. There, we provide a WKB analysis (before caustics), for cubic, defocusing nonlinearities.

All these results are valid in any space dimension.

Travelling waves for the Gross-Pitaevskii equation. **Philippe Gravejat** (Université de Paris-Dauphine, France) IC/MT541/025

Our talk is devoted to some recent results about the travelling waves for the Gross-Pitaevskii equation. This equation, which is written as:

$$i\partial_t u = \Delta u + u(1 - |u|^2)\,,$$

for a function $u : \mathbb{R}^N \mapsto \mathbb{C}$, is a model for Bose-Einstein condensation, superfluidity or nonlinear optics. The travelling waves are the solutions of the form

$$u(t,x) = v(x_1 - ct, \ldots, x_N)\,,$$

for some speed $c \geq 0$. Such solutions are supposed to play an important role in the long-time dynamics of the Gross-Pitaevskii equation.

In a series of papers, C.A. Jones, S.J. Putterman and P.H. Roberts investigated both formally and numerically their existence and qualitative properties, which raised a lot of interesting questions. Thus, we present some recent results which confirm some of the predictions formulated by C.A. Jones, S.J. Putterman and P.H. Roberts. In particular, we focus on existence and non-existence results, and the asymptotics of the travelling waves.

IC/MP141/042: Navier-Stokes equations and related topics.

Organiser: Alex Mahalov (Arizona State University, USA)
Co-organiser: Yoshikazu Giga (University of Tokyo, Japan)

The proposed minisymposium will focus on recent advances in the mathematical theory of Navier-Stokes equations with applications to geophysical flows. The topics will include: long time behaviour and global regularity, problems with almost periodic initial data, rotating fluids, boundary layer problems in geophysics and other related topics.

Stability of the Ekman spiral. **Matthias Hieber** (TU Darmstadt, Germany) IC/MT4346/042

In this talk we consider the question whether the Ekman spiral on the halfspace is stable under L^2-perturbations. We prove in particular that the Ekman spiral is linearly stable in the L^2-setting provided the associated Reynoldsnumber is small enough.

Rotating fluids with free boundary. **Jürgen Saal** (Universität Konstanz, Germany) IC/MT4351/042

Motivated by various applications in Geophysics (e.g., boundary layer problems) and technology (e.g., spin-coating processes) we study the free boundary problem for the Navier-Stokes equations with rotation. We will present an approach which is based on a reduction to a quasilinear system with dynamic boundary conditions. A major difficulty is to handle the corresponding boundary symbols, which look rather complicated and are nonhomogeneous in space and time. Here we apply methods relying on maximal regularity and the Newton-polygon in order to prove the wellposedness of a suitable linearization. This leads to a local-in-time existence result for the nonlinear problem. This is a joint project with R. Denk, M. Geissert, M. Hieber, and O. Sawada.

On the stationary Navier-Stokes flow with Coriolis force term. **Shin'ya Matsui** (Hokkaido Information University, Japan) IC/MT4698/042

From a meteorological point of view, if Coriolis parameter Ω is sufficiently large, flow will be independent of vertical direction asymptotically, that is 3 dim. flow will close to 2 dim. flow as $|\Omega| \to \infty$. This phenomena is called the Taylor-Proudman theorem. Our main purpose is to study this singular perturbation problem.

In my talk I will give the following results. For a fixed Ω, we obtained several unique existence theorems of the Cauchy problem and boundary value problem ($\mathbb{R}^3_+$) in some function spaces which include periodic functions, almost periodic functions and some L^∞ functions. After this I will discuss some asymptotic behavior of stationary velocity field in $L^2(D)$ as $\Omega \to \infty$.

My talk is based on joint works with Prof. Y. Giga (University of Tokyo, Japan), Prof. K. Inui (Keio University, Japan), Prof. A. Mahalov (Arizona State University, USA) and Prof. J. Saal (University of Konstanz, Germany).

Bursting dynamics of the 3D Euler equations in cylindrical domains. **Basil Nicolaenko** (Arizona State University, USA), Alex Mahalov (Arizona State University, USA) IC/MT4703/042

A class of three-dimensional initial data characterized by uniformly large vorticity is considered for the 3D incompressible Euler equations in bounded cylindrical domains. The fast singular oscillating limits of the 3D Euler equations are investigated for parametrically resonant cylinders. Resonances of fast oscillating swirling Beltrami waves deplete the Euler nonlinearity. These waves are exact solutions of the 3D Euler equations. We construct the 3D resonant Euler systems; the latter are countable uncoupled and coupled $SO(3;\mathbf{C})$ and $SO(3;\mathbf{R})$ rigid body systems. They conserve both energy and helicity. The 3D resonant Euler systems are vested with bursting dynamics, where the ratio of the enstrophy at time $t = t^*$ to the enstrophy at $t = 0$ of some remarkable orbits becomes very large for very small times t^*; similarly for higher norms $\mathbf{H}^s$, $s \geq 2$. These orbits are topologically close to homoclinic cycles. For the time intervals where $\mathbf{H}^s$ norms, $s \geq 7/2$ of the limit resonant orbits do not blow up, we prove that the full 3D Euler equations possess smooth solutions close to the resonant orbits uniformly in strong norms.

On a linearized operator of the equation for Burgers vortices. **Yasunori Maekawa** (Hokkaido University, Japan) IC/MT4905/042

Burgers vortices have been used as a model which expresses concentrated vorticity fields in turbulence. Several numerical results indicate that as the vortex Reynolds number is increasing, the associated Burgers vortex becomes more radially symmetric and has simpler structures. The purpose of this talk is to give a mathematical explanation for these numerical observations by studying a linearized operator of the equation for Burgers vortices.

IC/MP4/043: Extended splitting methods for partial differential equations: theory and application.

Organiser: Juergen Geiser (Humboldt-Universität zu Berlin, Germany)

In the last years different decomposition methods have played an important role in the numerical solution of differential equations. Since the pioneer work on time splitting methods like ADI and exponential splitting formulae, many new concepts and strategies have been developed and utilized. The adaptive methods in the area of the Splitting methods associated with finite differences, finite elements, or adaptations have been used widely and have been shown to have powerful capabilities in solving different differential equation problems in various applications. The aim of this special issue is to highlight the new developments in the area. It will contain articles presenting the latest trends and research results in topics including, but not limited to:

- splitting for higher efficiency and accuracy;
- splitting for non-linear differential equations;
- stability and convergence of splitting methods;
- iterative and adaptive splitting methods;
- splitting methods in parallel and quantum computations.

We would like to bring experts in theory and application together and discuss the recent development and the possible future works.

Nonlinear iterative operator-splitting methods and applications for nonlinear parabolic partial differential equations. **Juergen Geiser** (Humboldt-Universität zu Berlin, Germany) IC/MT5/043

In this paper we concentrate on nonlinear iterative operator-splitting methods for nonlinear differential equations. The motivation arose from decoupling nonlinear operator equations in simpler operator equations. The decomposition in simpler equations allow to apply adaptive time-discretisation methods in each underlying time-scale. Therefore one can solve the equations more effectively and accurate. The underlying coupling of the splitting method is fulfilled with a relaxation, coming from the results of the previous time-steps. the adapted problems. We consider the consistency and stability analysis of the nonlinear iterative operator splitting method. The consistency analysis is based on linearisation An *a priori* error estimates is derived for the linearised case. Finally we discuss the iterative operator-splitting methods for the applications to multi-physics problems.

Numerical simulation of 2D wave-equations via split sine and cosine schemes. **Qin Sheng** (Baylor University, USA) IC/MT4163/043

The problem is motivated form a realistic problem in seismic sources and waves. The underlying wave equation can be treated as a dispersive nonlinear partial differential equation which allows soliton-type solutions. We present a sine- and cosine-splitting of the basic equation; see[1]. With a semi-discretisation we arrive at a system of second-order nonlinear ordinary differential equations. By the traditional sequential splitting in linear manner we obtain locally one-dimensional problems. A further modification, the so-called iterative-splitting method, is presented as an alternative approach which has greater accuracy; see[2]. The underlying numerical stability is discussed. Numerical applications are given for demonstrations. Finally we discuss the extension to other multi-dimensional nonlinear wave simulations.

[1] Q. Sheng, A.Q.M. Khaliq, D.A. Voss; Numerical simulations of two-dimensional sine-Gordon solitons via a split cosine scheme. Mathematics and Computers in Simulations, Vol. 68, pp.335–373, 2005.

[2] J. Geiser and S. Nilsson; Seismic sources and waves using iterative operator splitting methods. Preprint, Humboldt Universität zu Berlin, Department of Mathematics, Germany. To be published, December 2006.

Time-parallel time integration methods for ODEs and PDEs. **Martin Gander** (Université de Genève, Switzerland) IC/MT1539/043

Time dependent problems are often solved using time marching schemes. Such schemes remain effective on parallel computers as long as each time step is costly enough for an effective parallelization in space. If not, parallelism in time could alleviate the situation, but is it possible to do useful computations at future time steps before the current time step results are known ?

I first present a historical overview of algorithms that were proposed over the last 40 years to obtain a certain amount of time parallelism. I will then introduce a general time domain decomposition method based on multiple shooting, which permits the parallel in time computation of solutions of time dependent problems. This time domain decomposition method contains more recent time parallel algorithms like the parareal algorithm. A convergence analysis reveals superlinear convergence of the method on bounded time intervals, and linear convergence on unbounded time intervals under certain conditions. I will illustrate the results with numerical experiments.

Efficient, adaptive and process-preserving modified Newton's method for solving reactive multicomponent transport problems. **Alexander Prechtel** (Universität Erlangen-Nürnberg, Germany) IC/MT2283/043

In the context of hydrogeochemical multicomponent transport problems coupled via reaction rates the fully implicit solution of the (discretized) problem can be computationally expensive, but it avoids the consistency errors inherent in the popular operator splitting approaches which seperate transport and reaction operators.

The efficiency of the process-preserving, globally implicit approach can be enhanced however by using as nonlinear solver a modified Newton's method.

Therefore the reaction network is analysed to neglect terms in the Jacobian whith the aim to decouple species equations on the level of the linear solver without deteriorating the quadratic performance of the global, process-preserving Newton iteration. This is possible, e.g., in the case of slow kinetics and/or small concentrations. A flexible list oriented, componentwise linear sparse matrix solver can adapt and change the coupling strategy of the groups of unknowns potentially in every iteration.

Numerical results of artificial and realistic case studies of reactive contaminant transport are presented that demonstrate the potential of the approach.

IC/MP4/043: Extended splitting methods for partial differential equations: theory and application. #2

Organiser: Juergen Geiser (Humboldt-Universität zu Berlin, Germany)

(For abstract, see session #1 above.)

A splitting moving-mesh method for 2D and 3D quenching and blow-up problems. **Ping Lin** (National University of Singapore) IC/MT3274/043

We study the numerical solution of multi-dimensional reaction-diffusion differential equations with a nonlinear force term over a rectangular domain. The equations may generate quenching or blow-up singularities depending on the force term. We will first focus on the quenching case to develop a variable temporal step splitting method on an adaptive moving mesh in space. The temporal and spatial adaptation is implemented based on parameterized arc-length estimations of the time derivative of the solution which will approach infinity when quenching takes place at certain spatial point. The multi-dimensional problem is split into a few one-dimensional problems so that the mesh moving can be done under a one-dimensional setting. The splitting procedure can also be parallelized so that the computational time is significantly reduced. The physical monotonicity of the solution and localized linear stability of this variable step adaptive scheme are analyzed. We also indicate that usual linearized stability analysis for the quenching problem is not appropriate when it is close to the quenching time. Thus a mathematically equivalent linearized problem is introduced to justify the stability. Finally we provide some numerical examples to demonstrate the viability and efficiency of the method for the quenching problem as well as other blow-up problems. We will also show the reduction of computational time when parallelly implementing the algorithm on a multi-CPU computer.

Stability and accuracy of higher-order operator splitting methods for parabolic equations. **Andrew Sornborger** (University of Georgia, USA) IC/MT3773/043

The Sheng-Suzuki theorem states that all exponential operator splitting methods of order greater than 2 must contain negative time integration. There have been claims in the literature that higher-order splitting methods for deterministic parabolic equations are unstable due to this fact. We show stability for a class of higher-order splitting methods for integrating deterministic parabolic equations. We note that problems with backwards time integration will still exist for stochastic integration methods for which information is lost and backward timesteps become ill-defined. Therefore, completely positive splitting methods, such as those developed by Chin, still have an important place. We present numerical results from first-, second-, third- and fourth-order methods showing that the error becomes increasingly small as the order increases.

On the local error of splitting approximations of reaction-diffusion equations with high spatial gradients. **Stéphane Descombes** (Ecole Normale Superieure de Lyon, France), Thierry Dumont (Université Claude Bernard Lyon 1 43 boulevard du, France), Violaine Louvet (Université Claude Bernard Lyon 1 43 boulevard du, France), Marc Massot (Ecole Centrale de Paris, France) IC/MT3784/043

In this talk we present some results on the approximation by splitting techniques of the ordinary differential equation $\dot{U} + AU + BU = 0$, $U(0) = U_0$ with A and B two matrices. We assume that we have a stiff problem in the sense that A is ill-conditionned and U_0 is a vector which is the discretization of a function with a very high derivative. This situation may appear for example when we study the discretization of a partial differential equation. We show some error estimates for two general matrices and in the stiff case, where the estimates are independent of U_0 and the commutator between A and B. As an example, a particular attention is paied to the study of the approximation of parabolic waves.

Propagation of high-intensity light in semiconductors. **Leonel Gonzalez** (General Dynamics Corporation, USA), Qin Sheng (Baylor University, USA), Shekhar Guha (Air Force Research Lab., Wright-Patterson AFB, USA) IC/MT4182/043

For photon energies below the bandgap, semiconductors exhibit high transparency. Propagation of light through this transparent medium can be described by a set of coupled, inhomogeneous, partial differential equations. For light collimated over the length of the sample, these equations can be written as:

$$\frac{\partial I}{\partial z} = -\left(1 + \frac{\Delta n}{n_0}\right)\left(\alpha I + \beta I^2 + \sigma_a N I\right) \quad (1)$$

$$frac\partial N\partial t = \frac{\beta I^2}{2h\nu} - \frac{N}{\tau} \quad (2)$$

$$Deltan = \sigma_r N + \frac{dn}{dT}\Delta T \quad (3)$$

$$frac\partial T\partial t = -\frac{1}{c_p}\frac{\partial I}{\partial z} \quad (4)$$

These equations describe the change in irradiance, I, as a function of the propagation direction z through the medium. The

irradiance source considered here is a laser having Gaussian spatial and temporal distributions, $I(r,t)$. Although the linear, single photon absorption α is typically low, under high irradiances, as during laser illumination, the contributions due to two photon absorption, β, and from free carriers, N, are significant.

A rate equation governs the generation of free carriers during the pulse. The carriers have a recombination lifetime, τ, which may be of the same order as the temporal duration of the laser pulse. Remaining equations describe the changes in refractive index, Δn and temperature, T. The parameter, σ_r is the refractive cross section of the free carriers, the thermo-optic coefficient of the medium is given by $\frac{dn}{dT}$, and the specific heat capacity is c_p. Not implicitly stated are the temperature dependencies of β, N, σ and τ.

To solve this set of coupled equations, a split-step finite difference scheme is used. For a given incident $I(r,t)$, the beam is propagated in space and time through the medium. At the output, the beam is temporally and spatially integrated yielding the total transmitted energy, which can be readily measured in the lab. Theoretical results and comparison with actual transmission measurements will be presented.

IC/MP2549/043: Dynamical models and game theory.

Organiser: Alberto Pinto (Universidade do Porto, Portugal)

See IC/MP339/015 on page 404 (Industrial Organization and Game Theory).

Edgeworthian economies. **Miguel Ferreira** (Universidade do Porto, Portugal) IC/MT881/043

General equilibrium theory assumes an interaction between individuals that is both global and anonymous. More, it presumes the existence of a "magic hand"which guides the way the market behaves. We study the effects of introducing a direct exchange mechanism between individuals in terms of dynamic models of an Edgeworthian exchange economy. We analyse the case where only two goods are traded and we assume random meeting between the market participants. We classify types of participants to study the effect of greed and we verify that greed is not always good and the minority wins more. We also present an evolutionary type model where consumers adapt to the market by temporally adjusting their individual preferences and their greediness.

Optimal investments to increase the market of the firms in repeated Cournot competition. **Bruno Oliveira** (Universidade do Porto, Portugal), Alberto Pinto (Universidade do Porto, Portugal), Fernanda Ferreira (Instituto Politecnico do Porto, Portugal), Flávio Ferreira (Instituto Politecnico do Porto, Portugal), Miguel Ferreira (Universidade do Porto, Portugal) IC/MT901/043

We present a deterministic dynamical model on the market size of Cournot competitions, based on Nash equilibriums of R&D investment strategies to increase the market of the firms at every period of the game. We study the transients and the asymptotic dynamics on the market sizes of the duopoly competition and their profound implications on the profit and persistence of the firms in the market. By adding uncertainty to the R&D investment strategies, we get a new stochastic dynamical model and we analyse the importance of the uncertainty to reverse the initial advantage of one firm with respect to the other.

International duopoly with unknown costs. **Hugo Sequeira** (Universidade do Porto, Portugal), Alberto Pinto (Universidade do Porto, Portugal), Fernanda Ferreira (Instituto Politecnico do Porto, Portugal) IC/MT905/015

Consider two identical countries. Each country has a government that chooses a tariff rate, a firm that produces output for both home consumption and export, and consumers who buy on the home market from either the home firm or the foreign firm. There is no other producer of this product for these two markets. We suppose that each firm has two different technologies, and chooses one of them following a common knowledge binary probability distribution. The utilization of one or the other technology affects the unitary production cost. The timing of the game is as follows: First, the governments simultaneously choose tariff rates. Then, both firms simultaneously choose quantities for home consumption and for export. We determine the Bayesian Nash equilibrium, and we analyse the advantage profits, for the firms and for the consumers, of the utilization of the technology with most expensive cost versus the utilization of the technology with cheapest cost. We also analyse the effect of the degree of differentiation of the goods on the equilibrium levels.

Flexibility and leadership advantages in a model with uncertain demand. **Fernanda Ferreira** (Instituto Politecnico do Porto, Portugal), Flávio Ferreira (Instituto Politecnico do Porto, Portugal), Alberto Pinto (Universidade do Porto, Portugal) IC/MT855/043

The Stackelberg model (1934) is one of the most widely-used models in industrial organization for analysing firms' behavior in a competitive environment. It studies the strategic situation where firms sequentially choose their output levels in a market. The question we ask is: Do first movers really have strategic advantage in practice? The belief of first-mover advantage was widely held among entrepreneurs and venture capitalists, but is now questioned by numerous practitioners. In this paper, we extend Liu's (2005) results by focus not only on the effects of the market demand uncertainty, but also on product differentiation, to explain the advantages and disadvantages of being the leading firm. Usually, the followers in markets get more market information than first movers before sinking their investments. In some industries that we consider to have fairly stable and predictable market demand, the pioneering firm tends to be the biggest player. However, if a market has a high degree of uncertainty, the followers can wait and see the customers' response to the new product introduced by the first movers, as well as move along the "differentiation curve" of innovation.

As in Liu's (2005) model, we consider that only the first mover (leading firm) faces demand uncertainty. The demand uncertainty is given by a random variable uniformly distributed, with mean μ and standard deviation σ characterizing the *demand uncertainty parameter* $\theta = (\mu + \sqrt{3}\sigma)/(\mu - \sqrt{3}\sigma)$. By the time the second mover chooses its output level, that uncertainty is resolved. Therefore, the leading firm possesses first-mover advantage, but the second mover enjoys an informational advantage because it can adjust the production level after observing the realized demand (flexibility). We study the advantages of flexibility over leadership as the degree $0 < \gamma \leq 1$ of the differentiation of the goods changes, where γ attains the value 1, if the goods are homogeneous, and tends to 0, if the goods are close to independent goods. We find explicit functions I_γ and J_γ, in terms of the degree of differentiation, characterizing the demand uncertainty parameter θ for which the leading firm looses its advantage for some realizations of the demand random variable. We show that the leading firm looses its advantage for high values of the demand intercept, if the demand uncertainty parameter θ is greater than I_γ, and for low values of the demand intercept, if the demand uncertainty parameter θ is greater than J_γ. Hence, for high values of the demand uncertainty parameter θ only in an intermediate zone of the realized demand does the first mover preserve its advantage.

IC/MP133/045: Free-boundary problems and their applications.

Organiser: Patrick Guidotti (UC Irvine, USA)
Co-organiser: Gieri Simonett (Vanderbilt University, USA)

This minisymposium features talks about both the theory of free-boundary problems and their applications to biology, chemistry and fluid dynamics.

Analytic solutions for the classical Stefan problem. **Gieri Simonett** (Vanderbilt University, USA) IC/MT3825/045

In this talk I will consider the classical one- or two-phase Stefan problem, where the free boundary is given as the graph of a function. Under mild regularity assumption on the initial data it will be shown that the problem admits a local solution that is analytic in space and time. The approach is based on optimal regularity results for an appropriate linearized problem, and on a scaling-translation argument in conjunction with the implicit function theorem.

Asymptotic behaviour of solutions of a multidimensional moving-boundary problem. **Joachim Escher** (Leibniz Universität Hannover, Germany) IC/MT1694/045

Of concern is a moving boundary problem modelling the growth of multicellular spheroids or in vitro tumors. This model consists of two elliptic equations describing the concentration of a nutrient and the distribution of the internal pressure in the tumor's body, respectively. The driving mechanism of the evolution is governed by Darcy's law. Finally surface tension effects on the moving interface counteract the internal pressure. Based on a centre manifold analysis, we prove that if the initial domain is sufficiently close to a Euclidean ball in the $C^{m+\mu}$-norm with $m \geq 3$ and $\mu \in (0,1)$, then the solution exists globally and the corresponding domains converge exponentially fast to some (possibly translated) ball, provided the surface tension coefficient γ is larger than a positive threshold value γ^*. In the case $0 < \gamma < \gamma^*$ the radially symmetric equilibrium centred at the origin is unstable.

A class of free-boundary problems with onset of a new phase. **Patrick Guidotti** (UC Irvine, USA) IC/MT2530/045

In this talk we shall address the well-posedness of a class of diffusive Free Boundary Problems characterized by the initial onset of a new phase. A novel regularity theory for linear singular elliptic and parabolic problems will be presented which is needed in the construction of a solution of the nonlinear coupled systems stemming from the considered class of Free Boundary Problems.

IC/MP3800/045: Free-boundary problems and their applications, II.

Organiser: Patrick Guidotti (UC Irvine, USA)
Co-organiser: Gieri Simonett (Vanderbilt University, USA)

This is an extension of the minisymposium IC/MP133/045 on page 340 since it has a total of 11 speakers.

On the regularity of a constrained system and applications to phase change problems. **Jose-Francisco Rodrigues** (Universidade de Lisboa, Portugal) IC/MT3903/045

The phase field approach for multi-phase systems leads to consider diffusion problems for the vector order parameter under constrains of the Gibbs simplex type. For certain potentials, these problems may be considered as special cases of a class of parabolic variational inequalities associated with convex sets defined by a system of obstacle type constraints. Under natural assumptions on these constraints, we use the Lewy-Stampacchia inequalities together with a simple iteration argument to show that the regularity of the solution is the same as the one corresponding to linear parabolic systems of second order. Special cases of constraints for ternary mixtures, for a system of two grains and for a diffuse interface model for simultaneous order-disorder and phase separation illustrate those estimates. This is a joint work with Lisa Santos.

Instability in a flame ball problem. **Luca Lorenzi** (Università degli Studi di Parma, Italy) IC/MT3833/045

In [1] the authors proposed a mathematical model to describe the combustion of a gaseous mixture with dust in a microgravity environment. Such a model gives rise to the following FBP in the unknowns γ, θ, u and the moving domain Ω:

$$\begin{cases} \gamma_t(t,x) = \dfrac{1}{\mathrm{Le}}\Delta\gamma(t,x), & t>0, \quad x \in \mathbb{R}^3 \setminus \overline{\Omega(t)}, \\ \gamma(t,x) = 0, & t>0, \quad x \in \Omega(t), \\ \vartheta_t(t,x) = \Delta\vartheta(t,x) + \beta u(t,x), & t>0, \quad x \notin \partial\Omega(t), \\ \Delta u(t,x) - 3\alpha^2 u(t,x) + \alpha\Delta\vartheta^4(t,x) = 0, & t>0, \quad x \notin \partial\Omega(t). \end{cases} \tag{1}$$

On $\partial\Omega(t)$, the following jump conditions are prescribed:

$$[\vartheta(t,\cdot)] = [\gamma(t,\cdot)] = 0, \qquad -\left[\frac{\partial\vartheta}{\partial\nu}(t,\cdot)\right] = \frac{1}{\mathrm{Le}}\left[\frac{\partial\gamma}{\partial\nu}(t,\cdot)\right], \qquad t>0, \tag{2}$$

$$\frac{1}{\mathrm{Le}}\left[\frac{\partial\gamma}{\partial\nu}(t,\cdot)\right] = F(\vartheta(t,\cdot)) \qquad u(t,\cdot)+\alpha\vartheta(t,\cdot) \ \text{ smooth}, \qquad t>0, \tag{3}$$

Moreover, at infinity it is assumed that

$$\gamma(t,x) \to \gamma_f, \quad \vartheta(t,x) \to \vartheta_f, \quad u(t,x) \to 0 \quad \text{as } |x| \to \infty, \qquad t>0. \tag{4}$$

The variables ϑ and γ correspond, respectively, to the temperature and the fuel mass fraction of the reactant, whereas u is a measure of the radiation flux. ϑ_f and γ_f denote the temperature and the mass fraction away in the fresh region. The parameters Le (Lewis number), α and β denote respectively the ratio between conductivity and diffusivity, the opacity of the medium and the ratio between the radiative and the diffusive flux. The space variable x belongs to $\mathbb{R}^3$, $\partial\Omega(t)$ is the free boundary variable corresponding to the flame front and $F(\vartheta(t,\cdot))$ is the reaction rate evaluated at $\partial\Omega(t)$, a simplified Arrhenius law, F being a smooth positive and increasing function. Finally, ν denotes the unit outward normal to $\partial\Omega(t)$.
As it has been shown in [1], Problem (1)-(4) admits steady state solutions (i.e., flame balls).
In this talk we show that, for particular values of the parameters α, β and Le, such flame balls are unstable with respect to smooth (and smooth) radial perturbations.
This is a joint work with V. Gujonne (Vrije Universiteit Amsterdam, The Netherlands)

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[1] V. Guyonne, J. Hulshof and J.B. van den Berg, *Flame balls for a free boundary combustion model with radiative transfer*, SIAM J. Appl. Math. (to appear)

The p-obstacle problem, some new perspectives. **Henrik Shahgholian** (Royal Institute of Technology (KTH), Sweden) IC/MT4491/045

TBA

Bifurcation of a free boundary problem for the Stokes equation: application to tumor growth. **Avner Friedman** (Ohio State University, USA) IC/MT1577/045

We introduce a free boundary problem for a system of PDEs consisting of the Stokes equation, several by parabolic equations and a diffusion equation. The system represents a growing tumor in fluid-like tissue. A biological parameter λ represents the cell-to-cell adhesiveness of the tumor cells. We show that a spherical stationary tumor is asymptotically stable if $\lambda > \lambda_0$ and is unstable if $\lambda < \lambda_0$. This is joint work with Bei Hu.

IC/MP133/045: Free-boundary problems and their applications. #2

Organiser: Patrick Guidotti (UC Irvine, USA)
Co-organiser: Gieri Simonett (Vanderbilt University, USA)

(For abstract, see session #1 above.)

Calculating deposit formation in the pipelining of waxy crude oils. **Antonio Fasano** (Università di Firenze, Italy) IC/MT1271/045

Analogue of the Rudin–Osher–Fatemi total variation model for fairing surfaces. **Matthew Elsey** (University of Michigan at Ann Arbor, USA), Andrea Bertozzi (University of California, Los Angeles, USA), Selim Esedoglu (University of Michigan, Ann Arbor, USA) IC/MT2595/045

Denoising of surfaces is an important problem in computer graphics applications. The goal is to remove noise and oscillations from the surface without rounding out important discontinuties in the normals (i.e. creases on the surface) such as the sharp edges of a cube. We show that the total variation based image denoising model of Rudin, Osher, and Fatemi has a very natural analogue for surface denoising.

Analysis and simulation of two-phase flows with soluble surfactant. **Dieter Bothe** (RWTH Aachen, Germany), Jan Pruess (Universität Halle–Wittenberg, Germany) IC/MT2680/045

Fluid particles like drops or bubbles play a prominent role in numerous applications. In such systems, at least one of the phases often contains surface active agents - unmeant as a contamination or by determined addition to increase the process efficiency - which preferentially adsorb at the interface due to minimization of free surface energy. The coverage with surfactant has a pronounced effect on the surface tension, hence on the stress balance at the interface which can lead to so-called Marangoni effects. This talk covers the mathematical modeling and analysis of such two-phase flows as well as their numerical simulation based on the Volume-of-Fluid (VOF) method.

Oil trapping in porous media. **Ben Schweizer** (Universität Basel, Switzerland) IC/MT1745/045

We consider the one-dimensional degenerate two-phase flow equations as a model for water-drive in oil recovery. The effect of oil trapping is observed in strongly heterogeneous materials with large variations in the permeabilities and in the capillary pressure curves. In such materials, a vanishing oil saturation may appear at interior interfaces and inhibit the oil recovery. We introduce a free boundary problem that separates a critical region with vanishing permeabilities from a strictly parabolic region and give a rigorous derivation of the effective conservation law.

IC/MP287/045: Free-boundary problem: moving interfaces and applications.

Organiser: Bo Su (Iowa State University, USA)

This minisymposium is to provide a forum to foster academic exchange and collaborations among active researchers in the area to address the fundamental problem in moving interface problem and their applications in material science, mathematical biology.

Bifurcation from stability to instability in a free boundary problem for elliptic–parabolic–hyperbolic system. **Avner Friedman** (Ohio State University, USA) IC/MT1576/045

We introduce a free boundary problem for a system of PDEs consisting of one diffusion equation, one parabolic equation, and several hyperbolic equations. The system represents tumor growth in a porous medium. The system has a family of stationary symmetry breaking bifurcation branches, with parameter μ representing the "aggressiveness" of the tumor. We study the asymptotic stability of the spherical solution, and determine the critical value of μ when the stability is lost. This is joint work with Bei Hu.

Gelification of waxy crude oils. **Antonio Fasano** (Università di Firenze, Italy), Mario Primicerio (Università degli Studi di Firenze, Italy) IC/MT3759/045

Mineral oils with a high content of heavy hydrocarbons are characterized by a peculiar thermodynamical behaviour influencing their rheology. Here we consider a saturated solution of one heavy in one light hydrocarbon, with the aim of describing two phenomena: (i) the segregation of solid crystals below some known temperature, (ii) the transition of the solution to a gel at an even lower temperature. When such phenomena take place in a prescribed thermal gradient they give raise to a complicated mass transfer process, due to the temperature dependence of the saturation concentration, with the formation of a gel on the cold wall and the formation of a region (necessarily unsaturated), completely depleted of crystals,

near the warm wall. Thus we have two free boundaries (the gelification front and the crystal depletion front). Two species are evolving: the solute concentration and the concentration of crystals. The crystals are supposed not to migrate and to exchange mass with the solution according to some (linear) kinetics. The solute can diffuse in the solution (i.e. prior to gelification), but is immobilized in the gel. Gelification occurs when the total concentration (solute+crystals) reaches a given temperature dependent threshold. Some results for the one-dimensional problem are presented.

Moving interfaces in heterogeneous oscillating media. **Panagiotis Souganidis** (University of Texas at Austin, USA) IC/MT3797/045

In this talk I will review recent results about the motion of interfaces in heterogeneous oscillating media. In particular I will present homogenization results for interfacial motions in periodic, almost periodic and random media.

Two-dimensional Riemann problems for systems of conservation laws. **Yuxi Zheng** (Pennsylvania State University, USA) IC/MT3793/045

We will report progress on the construction of solutions to the Riemann problem for the Euler system in 2-D and other systems such as the pressure gradient system. The results will include the interaction of binary planar waves, shock reflection on ramps, and others.

IC/MP287/045: Free-boundary problem: moving interfaces and applications. #2

Organiser: Bo Su (Iowa State University, USA)

(For abstract, see session #1 above.)

Continuity of the saturation for the Buckley–Leverett system. **Emmanuele DiBenedetto** (Vanderbilt University, USA), Vincenzo Vespri (Università degli Studi di Firenze, Italy), Ugo Gianazza (Università degli Studi di Pavia, Italy) IC/MT4414/045

We establish local continuity of the saturation for the Buckley-Leverett system of two immiscible fluids in a porous medium, with no assumption on the behavior of the pressure near the interfaces.

The sub-elliptic obstacle problem: $C^{1,\alpha}$ regularity of the free boundary in Carnot groups of step two. **Donatella Danielli** (Purdue University, USA) IC/MT4767/045

The sub-elliptic obstacle problem arises in various branches of the applied sciences, e.g., in mechanical engineering and robotics, mathematical finance, image reconstruction and neurophysiology. In recent work by Danielli, Garofalo and Salsa, it was proved that weak solutions to the sub-elliptic obstacle problem in a Carnot group belong to the Folland-Stein (optimal) Lipschitz class $\Gamma_l^{1,1}oc$ (the analogue of the well-known $C_l^{1,1}oc$ interior local regularity for the classical obstacle problem). However, the regularity of the free boundary remained a challenging open problem. In this talk we will show that, in Carnot groups of step r = 2, the free boundary is (Euclidean) $C^{1,\alpha}$ near points satisfying a certain thickness condition. This constitutes the sub-elliptic counterpart of a celebrated result due to Caffarelli.

On the regularity of the free boundary for the classical Stefan problem. **Gieri Simonett** (Vanderbilt University, USA) IC/MT4469/045

The regularity of the temperature and the free boundary for the Stefan problem has attracted much attention over the last 3 decades or so.

In this talk I will consider the classical one- or two-phase Stefan problem where the free boundary is represented as the graph of a function.

Under mild regularity assumptions on the initial data it will be shown that the problem admits a local solution that is analytic in space and time.

The approach is based on optimal regularity results for a linearized problem, and on a scaling-translation argument in conjunction with the implicit function theorem.

Front propagation in polymer crystallization. **Bo Su** (Iowa State University, USA) IC/MT1180/045

The aim of this talk is to show the global existence of weak solutions for a moving boundary problem arising in the non-isothermal crystallization of polymers. The main features of our works are (i) the moving interface is shown to be of co-dimension one; (ii)finite Hölder continuous propagation speed yields an intrinsic estimate of finite co-dimension one Hausdorff measure of the moving interface for every time t in two space dimension; (iii) based upon (ii), we prove Hölder continuity of the temperature u by a decomposition argument.

IC/MP317/046: Control problems for fluidodynamic models.

Organiser: Fabio Ancona (Università di Bologna, Italy)
Co-organiser: Benedetto Piccoli (Consiglio Nazionale delle Ricerche, Italy)

The theory of weak solutions of hyperbolic conservation laws received many foundamental contributions in the last years. In particular, the well-posedness theory for the Cauchy problem and for the mixed initial-boundary value problem is now well established in the case of systems in one space dimension. On the other hand, the study of these equations from the point of view of control theory is still at an early stage. The interest on such problems is motivated by applications to traffic flow models, multicomponent chromatography, as well as in problems of oil resevoir simulation and gas dynamic. Another related interesting area of research regards the control of equations over networks, to address application domain as car traffic flow, telecommunication, irrigation channels, etc.

When studying the effect of the boundary data treated as controls acting on the solutions of a conservation law one cannot expect to achieve in general complete controllability results within the space of discontinuous weak solutions, due to the particular wave-front structure of the solutions of such systems. It is then more appropriate to consider the problem of asymptotic stabilization of an hyperbolic system with boundary controls. Of particular interest for applications are general boundary controllability and stabilizability problems where the control acts only on some of the boundary conditions.

Another relevant direction in which it is being pursued the investigation of hyperbolic control problems is the study of necessary conditions for the optimality of a weak solution where the controls may act through the boundary conditions as well as through the source term of the balance laws. Here, the

main source of difficulties stems from the fact that the *input-to-trajectory map* that associates to a given control the corresponding solution may not be differentiable in any natural Banach space. For this reason to tackle such problems it has been crucial to introduce a suitable variational structure on the flow generated by conservation laws.

On boundary control for hyperbolic conservation laws. **Fabio Ancona** (Università di Bologna, Italy) IC/MT1062/046

We are concerned with the effect of boundary conditions on the solution of an hyperbolic system of conservation laws in one-space variable, from the point of view of control theory. Namely, given a fixed initial condition, we assume that the evolution of the system can be affected by an external controller acting through the boundary conditions and thus we shall regard the boundary data (or a partial number of their components) as boundary input controls. We will discuss some results concerning the finite time exact controllability and the asymptotic stabilizzability of the system relative to general boundary conditions. Moreover, we shall address the problem of determining an optimal solution of an hyperbolic system of balance laws relative to certain classes of cost functionals with boundary or distributed controls.

Control of the Camassa–Holm equation. **Olivier Glass** (Université Paris VI, France) IC/MT2647/046

The Camassa-Holm equation is a model of unidirectional waves at a free surface under the influence of gravity. We consider this equation in the circle $\mathbb{S}$, with a distributed control in a subdomain ω: for (t,x) in $[0,T]\times\mathbb{S}$,

$$u_t - u_{txx} + 2\kappa u_x + 3uu_x = 2u_x u_{xx} + uu_{xxx} + g(t,x)\mathbf{1}_\omega(x).$$

We study the controllability and the stabilization problems via the control g.

Controllability of the KdV equation. **Sergio Guerrero Rodríguez** (Université Paris VII, France) IC/MT2224/046

We present some controllability results concerning the linear KdV equation:

$$u_t+\nu u_{xxx}+Mu_x = 0 \quad (t,x)\in(0,T)\times(0,1),\ u(0,x)=u_0 \quad x\in(0,1)$$

In a first result we prove the null controllability of this equation for any $u_0 \in L^2(0,1)$ and $u(t,1) = u_x(t,1) = 0$. In a second result, we prove that whenever $T > C/|M|$ with C large but independent of M, the cost of the null controllability of the previous equation (same notion as above) is bounded with respect to ν as long as ν is small enough.

As a consequence of the previous results, we deduce an exact controllability result for the same equation and some local controllability results for the KdV (nonlinear) equation.

Asymptotic stabilization of one dimensional hyperbolic conservation laws. **Andrea Marson** (Università degli Studi di Padova, Italy), Fabio Ancona (Università di Bologna, Italy) IC/MT1829/046

Consider a strictly hyperbolic system of conservation laws in one space dimension on the interval $]0,1[$

$$\partial_t u + \partial_x f(u) = 0\,, \qquad u\in\mathbb{R}^n\,, \quad x\in]0,1[\,. \tag{1}$$

The main assumption is that the eigenvalues $\lambda_1(u),\dots,\lambda_n(u)$ of $Df(u)$ are bounded away from zero

$$\lambda_1(u) < \cdots < \lambda_p(u) < 0 < \lambda_{p+1}(u) < \dots \lambda_n(u)\,.$$

Moreover, we assume that the classical Lax conditions on genuine nonlinearity or linear degeneracy of the characteristic fields hold. Let an initial condition $u(0,x) = u_0(x)$ be given, together with a couple of boundary conditions at $x = 0$ and $x = 1$

$$b_0(u(t,0)) = 0\,, \qquad b_1(u(t,0)) = g(\alpha(t)) \in \mathbb{R}^p\,. \tag{2}$$

Here b_0, b_1 and g are smooth functions and $\alpha = \alpha(t) \in \mathbb{R}^k$, $n - p \le k \le p$, is a control function. It is well known that in general we can not obtain any result controllability in finite time [1]. Hence, we turn our attention to the problem of stabilizing the system around an equilibrium, i.e. a state $\tilde{u} \in \mathbb{R}^n$ such that

$$b_0(\tilde{u}) = 0\,, \qquad b_1(\tilde{u}) = g(\tilde{\alpha}) \quad \exists\tilde{\alpha}\in\mathbb{R}^k\,.$$

Provided the initial datum u_0 is sufficiently close to $\tilde{u}$ in L^∞ norm, and assuming that $\operatorname{rank} Dg(\alpha) = k$ for any α and other technical hypotheses on b_0 and b_1, we construct a control α and sequence of front tracking approximations converging to a solution $u = u(t,x)$ of (1)-(2) that approaches $\tilde{u}$ uniformly (in x) as $t \to +\infty$.

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IC/MP317/046: Control problems for fluidodynamic models. #2

Organiser: Fabio Ancona (Università di Bologna, Italy)
Co-organiser: Benedetto Piccoli (Consiglio Nazionale delle Ricerche, Italy)

(For abstract, see session #1 above.)

Traffic-like models for supply chains. **Pierre Degond** (Université Paul Sabatier Toulouse III, France) IC/MT793/046

We consider a supply chain consisting of a sequence of buffer queues and processors with certain throughput times and capacities. Based on a simple rule for releasing parts; i.e., batches of product or individual product items, from the buffers into the processors we derive a hyperbolic conservation law for the part density and flux in the supply chain. The conservation law will be asymptotically valid in regimes with a large number of parts in the supply chain. Solutions of this conservation law will in general develop concentrations corresponding to bottlenecks in the supply chain.

(Joint work with C. Ringhofer and D. Armbruster (Arizona State University

Optimal control of flows in 1D networks. **Günter Leugering** (Universität Erlangen–Nürnberg, Germany) IC/MT1783/046

We consider optimal control problems for flows in networked domains, like gas-, water- or traffic networks. In particular we consider the control of traffic on road networks and water flow in sewer- or irrigational systems. We first provide the mathematical modeling, in particular with regard to multiple joints, and review results on wellposedness and controllabililty. We then look into constrained optimal control problems for such transportation networks and provide numerical evidence. We further discuss problems of homogenization of some linearized models on periodic subgraphs.

Compactly-supported solutions of Euler equations. **Camillo De Lellis** (Universität Zürich, Switzerland) IC/MT4311/046

In a recent joint work with Laszlo Szekelyhidi we apply techniques of differential inclusions to construct distributional solutions of the 2-d Euler equations which are compactly supported in space and time. Such examples were first given in a pioneering work of Scheffer and later on by Shnirelman with a different construction.

We improve these two results from several points of view. First of all, in their examples the velocity is L^2 in time and space, and hence it does not belong to the naturaly energy space, whereas our construction yields bounded velocity and bounded pressure. Second, our proof is much shorter and quite elementary. Finally, though at a first sight Shnirelman's and Scheffer's constructions seem quite different, our approach gives a bridge between them.

IC/MP682/046: Conservation laws with discontinuous flux.

Organiser: Raimund Bürger (Universidad de Concepción, Chile)
Co-organiser: Kenneth Karlsen (Universitetet i Oslo, Norway)

Conservation laws and related equations, such as degenerate parabolic equations, having a discontinuous flux appear in several mathematical models in the applied sciences and engineering, such as clarifier–thickener models, traffic flow and multiphase flow through heterogeneous porous media. They are equally of theoretical interest.

The basic mathematical problem is that the well-posedness of these equations does not emerge straightforwardly as a limit case of the standard entropy solution theory of conservation laws with a flux that depends continuously on the spatial variable. In particular, there is no unique concept of admissibility conditions a jump of the solution across a jump of the flux (with respect to the spatial variable) needs to satisfy. For example, in applications of two-phase flow through a heterogenous porous medium, undercompressive jumps are not admissible, while the nature of the flux discontinuity in a clarifier–thickener model compels them in many situations.

A recent trend in dealing with this problem is the adaptation of these admissibility conditions to the physics of the underlying model considered. Moreover, most admissibility concepts are supported by a provably convergent numerical scheme.

In this minisymposium, we intend to exchange the latest developments in the area of conservation laws with discontinuous flux, which has attracted recent interest and generated a considerable number of contributions from researchers worldwide.

The Dirichlet problem for scalar conservation laws with discontinuous fluxes in several space dimensions. **Julien Jimenez** (Université de Pau et des Pays de l'Adour, France), Laurent Levi (Université de Pau et des Pays de l'Adour, France) IC/MT3629/046

We carry out the mathematical analysis of a quasilinear first-order hyperbolic equation set in the hypercube $\Omega =]-1,1[^n$. The problem can be read as follows for any positive and finite T: Find $u \in L^\infty(]0,T[\times\Omega)$ such that

$$\begin{aligned} \frac{\partial u}{\partial t} + \mathrm{div}(\mathbf{B}(x)g(u)) + f(t,x,u) &= 0 \text{ in }]0,T[\times\Omega, \\ u(0,.) &= u_0 \text{ on } \Omega, \\ u &= 0 \text{ on (a part of) }]0,T[\times\partial\Omega, \end{aligned}$$

where the vector field $\mathbf{B} = (B_1, ..., B_n)$, is such that only one of its components, named B_k, is discontinuous across the fixed hyperplane $[x_i = 0]$. We first provide the definition of a weak entropy solution for this equation. As we suppose that the convection term is *genuinely nonlinear*, we can define strong traces of an entropy solution at left and right of $[x_i = 0]$. This way the uniqueness property is obtained through the method of doubling variables and thanks to a Rankine–Hugoniot condition along the discontinuity.

We investigate two methods in order to obtain an existence result. The first one is based on a regularization of the component B_k while in the second one, we consider a vanishing viscosity method that consists in studying the limit when ϵ goes to 0^+ of the sequence $(u_\epsilon)_{\epsilon>0}$ of solutions to the diffusion problems:

$$\begin{cases} \dfrac{\partial u_\epsilon}{\partial t} + \mathrm{div}(\mathbf{B}(x)g(u_\epsilon)) + f(t,x,u_\epsilon) = \epsilon\Delta u_\epsilon \text{ in }]0,T[\times\Omega, \\ u_\epsilon(0,.) = u_0 \text{ on } \Omega, \\ u_\epsilon = 0 \text{ on }]0,T[\times\partial\Omega. \end{cases}$$

These results can be extended when the discontinuity of B_k occurs along a hypersurface.

A Riemann solver approach for conservation laws with discontinuous flux. **Andrea Terracina** (Università degli Studi di Roma "La Sapienza", Italy) IC/MT3652/046

We consider an hyperbolic scalar conservation laws with discontinuous flux of the following type

$$u_t + \big(H(x)f(u) + (1-H(x))g(u)\big)_x = 0 \quad \text{in } \mathbb{R}\times(0,T), \quad u(x,0) = u_0(x) \text{ in } \mathbb{R}\times\{0\},$$

where $f(u)$ and $g(u)$ are regular and concave and H is the Heaviside function. There are different applications in which this problem arises. In particular we are motivated from considering a fluidodynamic description for traffic flow on a simple road network, composed by two roads connected together by a junction (see[4]). This kind of problem was studied in literature see for example [1]–[7]. In particular in [2] and in [7] are given different formulations that in general characterize different solutions for this problem.

In [1,5], using different techniques, it was proved that it is possible to consider infinite class of entropy solutions and for each of these there is stability in L^1 respect to initial data. More precisely in [5] we observe that a concept of solution is uniquely characterized if we decide how to solve the Riemann problem. In this sense we give a formulation for the problem depending on that Riemann solver assuming that almost everywhere the traces $(u(0-,\cdot), u(0+,\cdot))$ are in equilibrium respect to the Riemann solver.

Existence is proved by a front tracking algorithm that takes in account the Riemann solver at the point $x = 0$ (see also [4]). Given a sequence of approximate front tracking solutions $\{u_n\}$ the main difficulty is to establish *a priori* BV estimate for the functions $f(u_n(\cdot,t))$, $g(u_n(\cdot,t))$ and $f(u_n(0+,\cdot))$.

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Semi-Godunov schemes for multi-phase flows in porous media. **Siddhartha Mishra** (Center of Mathematics for Appications, University, Norway), Kenneth Karlsen (Universitetet i Oslo, Norway), Nils Risebro (Universitetet i Oslo, Norway) IC/MT2698/046

In this talk, we consider three phase flows in porous media which arise while modeling petroleum reservoir simulation. The three phases are gas, oil and water. These models involve systems of two conservation laws which have a very complicated wave structure and are in general non-strictly hyperbolic. We design and implement finite volume schemes of the Godunov type which are based on a local decomposition of the system into a sequence of scalar conservation laws with discontinuous coefficients. These numerical schemes are very easy to implement and donot use the wave structure of the full system. Numerical examples illustrating the efficiency of the proposed method are presented.

A difference scheme for an inhomogeneous traffic model. **John Towers** (MiraCosta College, USA), Raimund Bürger (Universidad de Concepción, Chile), Kenneth Karlsen (Universitetet i Oslo, Norway) IC/MT2975/046

Our contribution discusses a simple finite difference scheme that we recently devised for kinematic flows modeled by conservation laws. We apply our scheme to a scalar conservation law modeling traffic flow on a highway. The flux has a discontinuous spatial parameter, which models for example a change in the number of lanes. We improve on our scheme by modifying it slightly at the interface where the jump occurs. This has the practical advantage of reducing or eliminating certain small spurious traveling waves that the original scheme produces. From a theoretical point of view, this modification implies that the scheme enforces a certain distinguished steady state solution. This allows one to prove that the limit of the scheme satisfies a so-called adapted entropy condition. We use this entropy condition to define a solution concept, and prove that our scheme generates approximations converging to such a solution.

IC/MP682/046: Conservation laws with discontinuous flux. #2

Organiser: Raimund Bürger (Universidad de Concepción, Chile)
Co-organiser: Kenneth Karlsen (Universitetet i Oslo, Norway)

(For abstract, see session #1 above.)

On adaptive multiresolution methods for hyperbolic conservation laws. **Margarete Domingues** (Instituto Nacional de Pesquisas Espaciais, Brazil) IC/MT3637/046

Adaptive strategies in space and time allow considerable speed up of finite volume schemes for conservation laws, while controlling the accuracy of the discretization. In the present talk, we present multiresolution techniques for finite volume schemes with explicit time discretization. An adaptive grid is introduced by suitable thresholding of the wavelet coefficients, which maintains the accuracy of the finite volume scheme of the regular grid. The number of costly flux evaluations is significantly reduced, together with the memory requirement, thanks to dynamic tree data structure. Further, speed-up is obtained by local scale dependent time stepping, i.e. on large scales larger time steps can be used without violating the stability condition of the explicit scheme. Furthermore, an estimation of the truncation error in time, using a Runge-Kutta-Fehlberg scheme, guarantees a control of the time step for a given precision. The accuracy and efficieny of the fully adaptive method is illustrated with applications.

Fully-adaptive multi-resolution schemes for strongly-degenerate parabolic equations with discontinuous flux. **Mauricio Sepúlveda** (Universidad de Concepción, Chile), Raimund Bürger (Universidad de Concepción, Chile), Kai Schneider (Université de Provence Aix-Marseille I, France), Ricardo Ruiz Baier (Universidad de Concepción, Chile) IC/MT3361/046

A fully adaptative numerical scheme for one-dimensional strongly degenerate parabolic equations with discontinuous flux is presented. The numerical scheme is based on a finite volume discretization using the approximation of Engquist-Osher for the flux and explicit time stepping. An adaptative multiresolution scheme with cell averages is then used to speed up CPU time and memory requirements, and we derive an optimal choice of the threshold in the adaptative multiresolution method. Applications to mathematical models of flocculated suspensions in a clarifier-thickener and traffic flow with driver reaction illustrate the efficiency of this method.

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Homogenization of two-phase porous-media flow with periodical heterogeneities. **Alexander Dressel** (Universität Stuttgart, Germany) IC/MT2917/046

The homogenization of periodical heterogenities in two-phase porous media flow is discussed, where water is injected into a porous medium with heterogeneous relative permeability. The flow is modelled as scalar conservation law with a Buckley-Leverett flux function having a discontinuous parameter. The analysis relies on appropriate energy estimates for the functional induced by the antiderivative of the discontinuous flux function in dependence of the spatial scale of capillarity and the microscale parameter.

Initial-data identification for conservation laws. **François James** (Université d'Orléans, France), Marie Postel (Université Pierre et Marie Curie, France) IC/MT3702/046

Identifying the initial data in a system of conservation laws is a major problem for instance in data assimilation. The problem can be formulated as the minimization of some cost function which compares the solution to some experimental observation. A natural idea is therefore to compute the gradient of the function, and this turns out to be very difficult when discontinuities are involved in the solution. Indeed the computations lead to linearize the original system, so that linear equations with discontinuous coefficients arise. In this talk, we shall on the one hand investigate the few available theoretical results in this direction, on the other hand present numerical strategies which give convenient results.

IC/MP418/046: Non-local conservation laws.

Organiser: Helge Holden (Norges Teknisk-Naturvitenskapelige Universitet, Norway)
Co-organiser: Kenneth Karlsen (Universitetet i Oslo, Norway)

In recent years nonlocal conservation laws have received a great deal of attention, both because they pose interesting mathematical and numerical problems and arise in a variety of different applications like shallow water waves, waves in compressible rods, radiating gases, and so forth. Typically, they take the form

$$u_t + uu_x + P_x = 0\,, \quad P = g \star h(u, u_x)\,, \quad t > 0\,,\ x \in \mathbb{R}\,,$$

where u denotes unknown function, g is a convolution kernel, often generated by the inverse of a differential operator, $\star$ denotes convolution in the spatial variable, and h is a given smooth function of u and u_x, typically linear or quadratic in its arguments. A frequently used example of a kernel g is $\frac{1}{2}e^{-|x|}$, which is the inverse of the operator $L = 1 - \partial_{xx}^2$, in which case the above equations takes the form of a hyperbolic–elliptic system:

$$u_t + uu_x + P_x = 0\,, \quad -P_{xx} + P = h(u, u_x)\,.$$

A few examples of nonlocal conservation laws are provided by the following list:

- Hunter–Saxton–Zheng equation:
$u_t + uu_x = \frac{1}{2}\int^x (u_x)^2 \mathrm{d}x$;
- Camassa–Holm equation:
$u_t + \gamma uu_x + P_x = 0\,, \quad -P_{xx} + P = \frac{1}{2}(3-\gamma)u^2 + \frac{1}{2}\gamma(u_x)^2$.
- Dai's rod equation: $u_t + \gamma uu_x + P_x = 0\,, \quad -P_{xx} + P = \frac{1}{2}(3-\gamma)u^2 + \frac{1}{2}\gamma(u_x)^2$.
- Degasperis–Procesi equation:
$u_t + uu_x + P_x = 0\,, \quad -P_{xx} + P = \frac{3}{2}u^2$.
- Burger–Poisson type model:
$u_t + uu_x + P_x = 0\,, \quad -P_{xx} + P = u$;
- RosenauŠs regularization model/radiating gas model: $u_t + uu_x + P_x = 0\,, \quad -P_{xx} + P = -u_x$.

Some of these equations (e.g., Camassa–Holm equation) possess truly remarkable properties such as an inifinite number of conserved integrals, a bi-Hamiltonian structure, and complete integrability, non-smooth solitary wave solutions, and wave breaking.

This session will present recent mathematical results (existence, uniqueness, stability, regularity, asymptotic/singular limit problems, etc.) on various types of nonlocal conservation laws. Additionally, the numerical treatment/analysis of these equations will be discussed. Finally, there will be presentation of examples where nonlocal conservation laws arise in the modelling of wave phenomena.

Initial boundary value problems for the Degasperis–Procesi equation. **Zhaoyang Yin** (Zhongshan University, PR China) IC/MT4699/046

This talk will address initial boundary value problems of the Degasperis–Procesi equation on the half line and on a compact interval. We first establish the local well-posedness for initial boundary value problems of the equation on the half line and on a compact interval, respectively. We then present some blow-up and global existence results for strong solutions. We finally investigate global and local weak solutions. One interesting result is that the corresponding strong solutions to the equation on the half line blow up in finite time provided the initial potential being negative is not identical with zero. The other one is that all global strong solutions to the equation on a compact interval blow up in finite time.

This work was done in collaboration with Joachim Escher and supported by the Alexander von Humboldt Foundation.

Non-local conservation laws for channel-porous media flow. **Steinar Evje** (Universitetet i Stavanger, Norway), Kenneth Karlsen (Universitetet i Oslo, Norway) IC/MT3801/046

We consider a mathematical model for fluid flow in a coupled channel-porous media system. The model is comprised of an integral equation representing unsteady 3-D porous media flow and the unsteady 1-D isothermal Euler equations representing flow in a channel-line. More precisely, the channel flow is described by the equations

$$\partial_t(A\rho_w) + \partial_s(A\rho_w u) = q_{\mathsf{M}}$$
$$\partial_t(A\rho_w u) + \partial_s(A\rho_w u^2) + A\partial_s p_w = q_{\mathsf{F}}, \qquad (s,t) \in [0, L_w] \times (0, T],$$

where s is position along the channel of length L_w and cross-sectional area A. $\rho_w(s,t)$ is fluid density, $u(s,t)$ fluid velocity, $p_w(s,t) = p(\rho_w(s,t))$ pressure, $q_{\mathsf{M}}(s,t)$ mass flow rate per unit wellbore length whereas $q_{\mathsf{F}}(s,t)$ represents frictional forces. The porous media flow may be described by the following integral representation

$$\rho_0(\mathbf{x}) - \rho(\mathbf{x}, t) = \int_0^t \int_0^{L_w} G(\mathbf{x}, \mathbf{X}_w(s'), t - t') q_{\mathsf{M}}(\mathbf{X}_w(s'), t') \|\mathbf{X}_w'(s')\|\, ds'dt',$$

where ρ_0 is initial density, $G(\mathbf{x}, \mathbf{X}_w(s'), t-t')$ is a kernel appropriate for porous media and $\mathbf{X}_w(s) = (x_w(s), y_w(s), z_w(s))$, $s \in [0, L_w]$ describes the channel-line. We are interested in simplified versions of this model that might shed light on some aspects of the full model. Particularly, we seek existence and uniqueness results, blow-up phenomena, and long-time behavior for these models.

Wave breaking in non-local dispersive wave equations. **Hailiang Liu** (Iowa State University, USA) IC/MT3852/046

The Korteweg–de Vries (KdV) equation is well known as an approximate model for small amplitude and long waves in different physical contexts, but wave breaking phenomena related to short wavelengths are not captured in. In this work we consider a class of nonlocal dispersive wave equations which also incorporates physics of short wavelength scales. The model is identified by a renormalization of an infinite dispersive differential operator, followed by further specifications in terms of conservation laws associated with the underlying equation. Several well-known models are thus rediscovered. Wave breaking criteria are obtained for several models including the Burgers-Poisson system, the Camassa-Holm type equation and an Euler-Poisson system. The wave breaking criteria for these models are shown to depend only on the negativity of the initial velocity slope relative to other global quantities.

Damping effects and nonlocal operators in radiation hydrodynamics. **Christian Rohde** (Universität Stuttgart, Germany) IC/MT4956/046

The dynamics of an inviscid radiating fluid can be described by the compressible equations of hydrodynamics coupled to an ensemble of linear transport equations for the direction dependent radiation intensity. Applications appear in astrophysics but also in down-to-earth problems like the simulation of flows in turbines. In these applications various limit regimes become important and give rise to consider a whole hierarchy of evolution equations. In particular the system depends on a parameter for the speed of light. Among others we consider the so-called nonrelativistic limit when this parameter tends to infinity. The limit regime is governed by a nonlinear but nonlocal conservation law. The existence of global weak solutions and -most notably- of classical solutions for small initial data is proven. We stress that solutions of standard nonlinear conservation laws develop shock singularities for general inital data. Finally we present numerical simulations for the limit conservation law which illustrates interesting radiation damping effects. This is joint work with Wen-An Yong and Nils Tiemann.

IC/MP272/047: Wave propagation in complex and random media.

Organiser: Peter Blomgren (San Diego State University, USA)

Over the last decade significant progress has been made in the theoretical understanding, numerical and simulation capabilities, as well as real-world applications of wavepropagation in complex/random media. Applications range from underwater acoustics, medical and industrial ultrasound, to electromagnetic imaging and communications using "smart antennas." In this minisymposium we focus on the state-of-the-art theory, simulations, and applications in the acoustic as well as electromagnetic regimes, with an emphasis on progress relating to time-reversal, imaging, communications and remote sensing.

Progress in computational wave propagation: simulated time-reversal and imaging in 3D random waveguides. **Peter Blomgren** (San Diego State University, USA) IC/MT2794/047

We quickly survey the development of computational wave propagation in random media during the last decade, and then focus on recent results of simulations in realistic size 3-dimensional wave guides where the propagation distance is in the hundreds or thousands of wavelengths. The recent computational studies are in the wireless (EM) regime, and we study the quality of communication in a multiple-in-single-out (MISO) TR-based communications system.

(Joint work with George Papanicolaou)

Propagation and detection in clutter. **Knut Solna** (University of California, Irvine, USA) IC/MT2814/047

We consider propagation in a cluttered environment. In the case with long range propagation and medium variations we discuss how the wave interacts with the medium. We also consider how scatterer detection performance is affected in such a noisy environment.

Pulse propagation and time reversal in random waveguides. **Josselin Garnier** (Université Paris VII, France) IC/MT1902/047

We consider pulse propagation in a random waveguide. We perform an asymptotic analysis based on separation of scales, when the propagation distance is large compared to the size of the random inhomogeneities, which have small variance, and when the typical wavelength is comparable to the scale of the inhomogeneities.

We study the asymptotic form of the joint distribution of the mode amplitudes at different frequencies. We derive from first principles an asymptotic deterministic system of time-frequency transport equations for the coupled mode amplitudes.

We apply the transport equations to study pulse spreading in a random waveguide and to show how randomness reduces time dispersion at the expense of having random fluctuations. We also apply them to analyze time-reversal in a random waveguide. We show that randomness enhances spatial refocusing and that diffraction-limited focal spots can be obtained even with small-size time reversal mirrors. However, statistical stability for narrowband refocused fields is achieved only for large-size time reversal mirrors. The mechanisms responsible for statistically stable refocusing in a random waveguide are clarified.

Work in collaboration with George Papanicolaou (Stanford University).

Direct-imaging algorithms for extended targets. **Hongkai Zhao** (University of California, Irvine, USA) IC/MT1630/047

I will present a few direct imaging algorithms for extended targets using both near and far field data. No forward problem or iterations are neended in our algorithms. Robustness with respect to both measurement noise and medium inhomogeneity will be shown. This is joint work with S. Hou, K. Huang, and K. Solna.

IC/MP272/047: Wave propagation in complex and random media. #2

Organiser: Peter Blomgren (San Diego State University, USA)

(For abstract, see session #1 above.)

Kinetic limits for wave equations in random media. **Lenya Ryzhik** (University of Chicago, USA) IC/MT2541/047

I will describe some of the results on the kinetic equations for the phase space wave energy density in random media. Such equations typically arise in the high frequency, long propagation distance limit. These results are a joint work with G. Bal and T. Komorowski.

Illumination design for imaging. **Chrysoula Tsogka** (University of Chicago, Greece) IC/MT2732/047

We consider array imaging in clutter with coherent interferometric techniques. We address the problem of optimal illumination and seek the input waveform using an optimality criterion that measures the quality of the resulting image. The robustness of the method is illustrated with several results.

This is joint work with Liliana Borcea and George Papanicolaou

Optimal waveform design for array imaging. **Liliana Borcea** (Rice University, USA) IC/MT2560/047

This talk is concerned with an inverse problem for the wave equation. More specifically, it considers coherent imaging of reflectors from measurements of the echoes at a remote array of transducers. The main question raised is how to design optimally the waveform used by the array to illuminate the reflectors, so that the image has the best resolution.

Imaging in random media. **George Papanicolaou** (Stanford University, USA) IC/MT3206/047

I will present a brief overview of array imaging methods when the medium between the object to be imaged and the array that is collecting the data is a random medium. This means that it is not known in detail but only statistically and through the array data. Imaging the object of interest cannot be done without some estimation of the properties of the random medium. What properties should be estimated and how? I will address this question and give some answers based on recent work on adaptive coherent interferometry done jointly with L. Borcea and C. Tsogka.

IC/MP308/047: Homogenization, inverse problems, and shape optimization.

Organiser: Eric Bonnetier (Université Grenoble I, France)
Co-organiser: Elena Cherkaev (University of Utah, USA)

Recent developments in homogenization, multiscale analysis, inverse problems, imaging of microstructured media, and shape optimization reveals that these fields share several fundamental concepts. For instance, asymptotic techniques in non-homogeneous media have fostered stable reconstruction algorithms in inverse problems. Similar asymptotics have led to new iterative methods in shape optimization. Homogenization results allowed to develop approaches to inverse or dehomogenization problems for materials with microstructure.

The minisymposium will focus on the interaction of ideas stemming from these areas.

Electrical impedance tomography with resistor networks. **Fernando Guevara Vasquez** (Stanford University, USA), Liliana Borcea (Rice University, USA), Vladimir Druskin (Schlumberger Ltd., USA) IC/MT1803/047

Electric impedance tomography consists in finding the conductivity inside a body from electrical measurements taken at its surface. This is a severely ill-posed problem: any numerical inversion scheme requires some form of regularization. We present inversion schemes that address the instability of the problem with a reduced model approach, where the reduced models are resistor networks that arise in the finite volumes discretization of the forward problem. Specifically, we consider finite volume grids of size determined by the measurement precision, but where the node locations are determined adaptively. We show that the model reduction problem of finding the smallest resistor network (of fixed topology) that can predict measurements of the Dirichlet-to-Neumann map is uniquely solvable for a broad class of measurements. We view the model reduction as a nonlinear map of the data. Numerical evidence suggests this map acts as an approximate inverse of the forward map. To image the conductivity we use this map as a preconditioner in a Newton type iteration. A priori information can be easily incorporated to the method.

On combining model reduction and Gauss–Newton algorithms. **Vladimir Druskin** (Schlumberger Ltd., USA), Mikhail Zaslavsky (Schlumberger Ltd., USA) IC/MT1605/047

We suggest an approach to speed up the Gauss-Newton solution of inverse PDE problems by minimizing the number of forward problem calls. The acceleration is based on effective incorporation of the information from the previous iteration via a reduced order model (ROM). It is designed with the help of Galerkin and pseudo-Galerkin methods for self-adjoint and complex symmetric problems respectively. The constructed ROM generates effective multivariate rational interpolation matching the forward solutions and the Jacobians from the previous iterations. Numerical examples for the inverse conductivity problem for the 3D Maxwell system show significant accelerations.

G-convergence and homogenization of a model of two-phase viscoelastic flows. **Alexander Panchenko** (Washington State University, USA) IC/MT2523/047

We study the system of balance equations modeling the flow of a two-phase, Kelvin–Voight viscoelastic material. We consider a sequence of highly oscillatory initial data, parametrized by a small parameter ε. The initial geometry is generic in the sense that periodicity or even random homogeneity are not assumed. Using G-convergence and oscillating test functions, we pass to the limit $\varepsilon \to 0$ and obtain an effective system of equations. These equations model a one-phase viscoelastic flow. The mass balance equation and convective terms in the momentum balance equation have the standard structure. The constitutive equation for effective stress contains a long memory term which is not present in the ε-problems.

Structural information of strongly heterogeneous two-component composites. **Christian Engstrom** (Universität Karlsruhe, Germany) IC/MT4993/047

For strongly heterogeneous two-component composites we address the inverse problem of estimating microstructural parameters from permittivity measurements. The dependence on the geometrical structure is reduced to the problem of calculating the moments of the measure in an integral representation of the effective permittivity. We present a method that uses measurement data at a set of distinct frequencies to calculated bounds on several moments, such as the volume fraction and the anisotropy of a composite. We show that this inverse homogenization method can be used even with a low number of data points and in the cases when the accuracy in the measurements is low. Furthermore, we use the microstructural information to tighten error bars on measurement data.

IC/MP308/047: Homogenization, inverse problems, and shape optimization. #2

Organiser: Eric Bonnetier (Université Grenoble I, France)
Co-organiser: Elena Cherkaev (University of Utah, USA)

(For abstract, see session #1 above.)

Inverse homogenization: can one hear the structure of composite materials?. **Elena Cherkaev** (University of Utah, USA) IC/MT2547/047

Inverse homogenization is a problem of deriving information about the microgeometry of composite material from its effective properties. The approach is based on reconstruction of the spectral measure in the analytic Stieltjes representation of the effective tensor of two-component composite. This representation relates the n-point correlation functions of the microstructure to the moments of the spectral measure, which contains all information about the microgeometry. The problem of identification of the spectral function from effective measurements in an interval of frequency has a unique solution, however the problem is ill-posed. The talk discusses several stabilization techniques as well as Pade approximations used to reconstruct the spectral function. Results of reconstruction of microstructural parameters are shown for visco-elastic composites and for composites of two materials with different complex permittivity. The reconstructed spectral function can be used to compute other effective parameters of the same composite; this gives solution to the problem of coupling of different effective properties of a two-component random mixture.

On de-homogenization of poroelastic materials . **Miao-jung Ou** (University of Central Florida, USA) IC/MT2818/047

In this talk, we present a de-homogenization scheme for inversion of microstructural informations from measurement data of effective stiffness moduli of a poroelastic composite with a band acoustic frequencies. The scheme is based on the integral representation formula which was first derived by Kantor & Bergman and further generalized by Ou & Cherkaev.

Periodic homogenization in Fourier space. **Niklas Wellander** (Swedish Defence Research Agency, Sweden) IC/MT2426/047

A two-scale Fourier transform for periodic homogenization in Fourier space is introduced. For any function f in $L^1(\mathbb{R}^n)$ and $\varepsilon > 0$ the *two-scale Fourier transform at the ε-scale* of f is defined by

$$\mathcal{F}_\varepsilon\{f\}(\xi, m) = \hat{f}_\varepsilon(\xi, m) = \int_{\mathbb{R}^n} f(x) e^{-2\pi i x\cdot\left(\xi+\frac{m}{\varepsilon}\right)} \mathrm{d}x\,,$$

for all $\xi \in \mathbb{R}^n, m \in \mathbb{Z}^n$. The corresponding inverse transform is given by

$$\mathcal{F}_\varepsilon^{-1}\{\hat{f}_\varepsilon\}(x) = \sum_{m\in\mathbb{Z}^n} \int_{\xi\in[-\frac{1}{2\varepsilon},\frac{1}{2\varepsilon}]^n} \hat{f}_\varepsilon(\xi, m) e^{2\pi i x\cdot\left(\xi+\frac{m}{\varepsilon}\right)} \mathrm{d}\xi\,.$$

The transform is applied to a standard periodic homogenization problem for homogenization in Fourier space. The transform is also used to define a two-scale transform (sometimes called periodic unfolding) and to Floquet–Bloch decompose differential operators.

The polarization tensor for irregular perfectly conducting inclusions. **Frédéric de Gournay** (Université de Versailles, France) IC/MT3322/047

We study how perturbations of the domain interferes with the solution of the Laplace equation with Dirichlet boundary conditions. The perturbations, in finite number, are allowed to be quite irregular. They may be of two kinds: Either they are a sequence of holes whose diameter (say smaller than ϵ) goes to zero. Or, they are perturbations of C^∞ holes, with the restriction that the pertubed holes contain the unperturbed ones, and that the distance between perturbed and unperturbed boundaries is smaller than ϵ. We show that the solution of the Laplace equation is differentiable with respect to ϵ in a weak sense. This work extends several cases of derivation with respect to the domain: the approach of Vogelius and Capdeboscq (who studied holes filled with weak material), the topological gradient (or bubble method) valid only for regular holes, and shape derivation techniques that are only valid for regular transport of a hole. Our method is based on energy estimates and therefore, may be quite easily extended to other elliptic operators.

IC/MP322/047: Nonlinear PDE techniques in imaging.

Organiser: Martin Burger (Universität Münster, Germany)
Co-organiser: Antonin Chambolle (École Polytechnique, France)

Imaging is a field of growing interest due to various important applications (e.g., in medicine and industry), which poses a lot of extremely challenging questions to applied and computational mathematics. Whereas linear filtering and PDE methods were and still are strongly for various tasks in imaging, there is a strong trend towards nonlinear PDE techniques nowadays, due to their superior capabilities to handle these tasks (such as segmentation, motion estimation, inpainting and even denoising). Celebrated examples of nonlinear PDE techniques are Perona–Malik filters and methods based on total variation and curvature.

The aim of this mini-symposium is to give a presentation of modern nonlinear PDE techniques (including second- and fourth-order PDE approaches) for several different tasks from several different perspectives. It includes speakers focusing on analysis, modelling, and computation, to highlight all of the different aspects. Moreover, two speakers are applied computer scientists bringing in an even more applied perspective of PDE techniques in imaging.

Non-linear regularization of irregular sampling problems in digital imaging. **Andrés Almansa** (Ecole Normale Supérieure de Cachan, France), Vicent Caselles (Universitat Pompeu Fabra, Spain), Gabriele Facciolo (Universitat Pompeu Fabra, Spain), Gloria Haro (University of Minnesota, USA), Bernard Rougé (Centre National d'Etudes Spatiales, France) IC/MT2368/047

We propose several algorithms to solve a problem in image restoration which considers several different aspects of it, namely: irregular sampling, denoising, deconvolution, and zooming. The first algorithm is based on an extension of a previous image denoising algorithm proposed by A. Chambolle using total variation, combined with irregular to regular sampling algorithms proposed by H.G. Feichtinger, K. Gröchenig, M. Rauth and T. Strohmer, and local constraints ideas from V. Caselles et. al. Then a few variants of total variation regularization, local constraints, and discretization techniques are considered in order further reduce the computational cost of the algorithm while at the same time better controling artifacts in coarsely sampled areas. Finally we present some experimental results and we compare them with those obtained with the algorithm proposed by K. Gröchenig et al.

How to discretize the total variation of an image?. **Lionel Moisan** (Universite Rene Descartes, Paris, France) IC/MT2790/047

The Total Variation (TV) has been introduced in the context of image restoration by Rudin, Osher and Fatemi 15 years ago as a Tikhonov-like regularization term more suitable to images than the classical H^1 norm. Since then, it has been used in many domains of image processing and analysis, including deblurring, blind deconvolution, zoom, inpainting, etc. Still recently it received a lot of attention both as the first component of Meyer's $u + v$ decomposition (and all following work), and because of the discover of new dual-based minimization algorithms (Carter, Chan-Golub-Mulet, Chambolle, ...). In this talk we study and compare possible discretizations of the total variation, and we show that finite differences are not very efficient, especially for small scales (pixel and sub-pixel scales). We then propose a new Fourier-based estimate (called spectral TV) that behaves much better in terms of grid invariance, isotropy, artifact removal, and sub-pixel accuracy, both as an estimate of the exact continuous TV and and as a control term (i.e. regularization term) for energy-minimization models based on TV minimization. We illustrate these properties with experiments, showing that the spectral TV significantly improves the quality of the results.

Solving the Chan–Vese model by a multi-phase level-set algorithm based on the topological derivative. **Lin He** (RICAM Linz, Austria), Stanley Osher (University of California, Los Angeles, USA) IC/MT4092/047

In this work, we specifically solve the Chan–Vese active contour model by multiphase level-set methods. We first develop a fast algorithm based on calculating the variational energy of the Chan–Vese model without the length term. We check whether the energy decreases or not when we move a point to another segmented region. Then we draw a connection between this algorithm and the topological derivative, a concept emerged from the shape optimization field. Furthermore, to include the length term of the Chan–Vese model, we apply a preprocessing step on the image by using nonlinear diffusion. We show numerical experiments to demonstrate the efficiency and the robustness of our algorithm.

PDEs in medical image reconstruction. **Frank Wuebbeling** (Universität Münster, Germany) IC/MT4185/047

While integral geometry techniques used to be the dominant tool in medical image reconstructions (in particular, in computed and emission tomography) in past years, the need for higher-precision and lower-dose modalities more and more require PDE methods which are capable of modeling the underlying physical processes more accurately.

Some examples include ultrasound tomography (governed by the Helmholtz equation in frequency domain or the wave equation in time domain), optical tomography (governed by the transport or diffusion equation, depending on the type of the underlying material, both in time and frequency domain) or high-precision Positron Emission Tomography (governed by the transport equation, taking scatter into account). Although the differential equations in these problems are linear, they usually lead to nonlinear inverse problems for a material parameter since coefficients and solutions to the PDEs both depend on the parameter, thus leading to large systems of bilinear equations.

Transferring the established ART-scheme from classical tomography to these non-(bi-)linear equations, we develop nonlinear ART, an adjoint method for the solution of nonlinear equations. Ultrasound tomography serves as an example for how this can be implemented in a very efficient way.

The method is applied to the modalities above, several examples are shown.

IC/MP322/047: Nonlinear PDE techniques in imaging. #2

Organiser: Martin Burger (Universität Münster, Germany)
Co-organiser: Antonin Chambolle (École Polytechnique, France)

(For abstract, see session #1 above.)

Mathematical aspects of the total variation approach to image restoration. **Vicent Caselles** (Universitat Pompeu Fabra, Spain) IC/MT1416/047

Image restoration (deconvolution and denoising) is an ill-posed problem usually solved with a regularization method. The use of total variation as a regularizing term was proposed by L. Rudin, S. Osher and E. Fatemi in 1992. In this model, to restore an image, one minimizes total variation under the constraints imposed by the image acquisition model. The corresponding Euler-Lagrange equation is a singular elliptic PDE involving the 1-Laplace operator. We study this PDE and its explicit solutions which lead to a series of geometric problems related to the characterization of calibrable sets. We interpret these results in terms of $u + v$ image decompositions in the sense of Yves Meyer. We also discuss the problem of image restoration in the case of irregularly sampled data.

Topological and variational properties of a model for the reconstruction of three-dimensional transparent images with self-occlusions. **Giovanni Bellettini** (Dipartimento di Matematica, Universita' di Roma To, Italy) IC/MT1593/047

We introduce and study a two-dimensional model for the reconstruction of a smooth generic three-dimensional scene E, which may handle the self-occlusions and that can be considered as an improvement of the 2.1D sketch of Nitzberg and Mumford. We characterize from the topological viewpoint the apparent contour of E, namely, we characterize those planar graphs G that are apparent contours of some scene E. Moreover, we show that if E and F are two of these scenes, then E and F differ by a global homeomorphism which is strictly increasing on each fiber along the direction of the eye of the observer. These two topological theorems allow to find the domain of the functional $\mathcal{F}$ describing the model. Compactness, semicontinuity and relaxation properties of $\mathcal{F}$ are then studied, as well as connections of our model with the problem of completion of hidden contours.

Work made in collaboration with V. Beorchia (Dipartimento di Matematica e Informatica, Università di Trieste, via Valerio 12/b, 34127 Trieste, Italy, E-mail: beorchia@units.it) and M. Paolini (Dipartimento di Matematica, Università Cattolica "Sacro Cuore", via Trieste 17, 25121 Brescia, Italy E-mail: paolini@dmf.unicatt.it).

Statistical shape influence in level-set segmentation. **Daniel Cremers** (Universität Bonn, Germany) IC/MT1654/047

Level-set methods have been developed to optimally partition a given image based on various assumptions about the intensity, color texture or motion of objects of interest. Nevertheless, most applications provide suboptimal segmentation results, as soon as these assumptions are not fulfilled – in particular if the input images are corrupted by noise, background clutter or partial occlusions of the objects of interest. In such cases, the segmentation results can be drastically improved by introducing prior shape knowledge into the segmentation process. I will present recent advances regarding the modeling of shape dissimilarity measures and their introduction into the segmentation process on a variational level. In particular, I will discuss the concept of *intrinsic alignment* to obtain invariance to certain group transformations, the concept of *dynamic labeling* to model the introduction of multiple competing shape priors, and the concept of *dynamical shape priors* which allows to statistically learn and impose information about temporal evolutions of implicit shapes. Respective parts of this work are based on collaborations with Nir Sochen, Christoph Schnoerr, Stanley Osher and Stefano Soatto.

A generalization of Cahn–Hilliard inpainting for gray-value images. **Carola-Bibiane Schönlieb** (Universität Wien, Austria), Martin Burger (Universität Münster, Germany) IC/MT1680/047

The Cahn-Hilliard equation has its origin in material sciences and serves as a model for phase separation and phase coarsening in binary alloys. A new approach in the class of fourth order inpainting algorithms is inpainting of binary images using the Cahn-Hilliard equation proposed in [1]. In this talk I will present a generalization of this fourth order approach for grayvalue images. This is realized by using subgradients of the total variation functional within the flow, which leads to structure inpainting with smooth curvature of level sets. I will present some numerical examples for this approach and analytic results concerning existence and convergence of solutions.

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IC/MP254/047: **Image processing based on partial differential equations.**

Organiser: Antonio Marquina (Departamento Matematica Aplicada, Universidad de, Spain)
Co-organiser: Xue-Cheg Tai (Universitetet i Bergen, Norway)

PDE methods in image processing have experienced an impressive growth along the last fifteen years as a consequence to the advances in technology of imaging. Those methods have been applied to several important problems like image restoration, segmentation, inpainting, registration, surface construction,... The purpose of this minisymposium is to present and discuss recent advances and various aspects of new developments in using numerical techniques for partial differential equations to analyze and process digital images.

High-order geometric motion of an interface induced by diffusing distance functions. **Yen-Hsi Tsai** (University of Texas at Austin, USA) IC/MT3358/047

We propose a stable and efficient algorithm that iterates the steps of obtaining short time solutions of a linear PDE and nonlinear operations that involve redistancing (distance reinitialization) in order to achieve high order geometric motions of an interface. Traditional threshold dynamic approaches typically require large kernel size for the high order motions of interest and are not suitable for grid based computations. In this talk, we show the derivation of our algorithm and discuss the consistency, stability, and implementation of this algorithm.

This is joint work with Selim Esedoglu and Steven Ruuth.

A comparison of total variation *optimization algorithms.* **Jérôme Darbon** (University of California, Los Angeles, USA), Sylvain Lefebvre (INRIA Rocquencourt, USA), Tony Chan (National Science Foundation, USA), Selim Esedoglu (University of Michigan, Ann Arbor, USA) IC/MT3696/047

This study copes with the comparison of some Total Variation (TV) optimization algorithms. It includes an Euler–Lagrange based algorithm, the dual approach of Chambolle and finally a graph-cut (i.e., a combinatorial) based one. So far the last one is the known as the fastest. The main interest of this work is that the Euler–Lagrange algorithm is also implemented on a Graphic Processor Unit (GPU). Using this GPU architecture, it is shown that the Euler-Lagrange version is a serious competitor to the graph-cut based one. Finally some deep theoretical links between graph-cuts and TV optimization are shown.

Level-set methods for watershed image segmentation. **Erlend Hodneland** (Universitetet i Bergen, Norway) IC/MT3440/047

In this study a marker-controlled and regularized watershed segmentation is proposed. Only a few previous studies address the task of regularizing the obtained watershed lines from the traditional marker-controlled watershed segmentation. In the present formulation, the topographical distance function is applied in a level set formulation to perform the segmentation, and the regularization is easily accomplished by regularizing the level set functions. Based on the well-known Four-Color theorem, a mathematical model is developed for the proposed ideas. With this model, it is possible to segment any 2D image with arbitrary number of phases with as few as one or two level set functions. The algorithm has been tested on real 2D fluorescence microscopy images displaying rat cancer cells, and the algorithm has also been compared to a standard watershed segmentation as it is implemented in MATLAB. For a fixed set of markers and a fixed set of challenging images, the comparison of these two methods shows that the present level set formulation performs better than a standard watershed segmentation.

A time-evolution model for total-variation-based blind deconvolution. **Antonio Marquina** (Departamento Matematica Aplicada, Universidad de, Spain) IC/MT1976/047

In this research work we study a model for blind deconvolution based on the minimization of the total variation functional ([5],[2],[3]) combined with the Bregman iterative refinement procedure. The Bregman iterative refinement procedure is a technique used to recover finer scales in total variation based image restoration methods, ([1],[4]). The model is written as a system of PDEs evolving in time the signal and the estimated kernel, integrating implicitely the Bregman iteration in the whole process. We propose an explicit scheme that recovers edges and textures from a blurry and noisy signal. Nu-

merical tests indicate that the iterative procedure is stable and converges very fast to the restored images from initial images convolved with Gaussian blur and contaminated with Gaussian white noise.

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IC/MP254/047: Image processing based on partial differential equations. #2

Organiser: Antonio Marquina (Departamento Matematica Aplicada, Universidad de, Spain)
Co-organiser: Xue-Cheg Tai (Universitetet i Bergen, Norway)

(For abstract, see session #1 above.)

Iteratively solving linear inverse problems under general convex constraints. **Luminita Vese** (University of California, Los Angeles, USA), Ingrid Daubechies (Princeton University, USA), Gerd Teschke (Zuse-Institut Berlin, Germany) IC/MT3074/047

We consider linear inverse problems where the solution is assumed to fulfill some general homogeneous convex constraint. We develop an algorithm that amounts to a projected Landweber iteration and that provides and iterative approach to the solution of this inverse problem. For relatively moderate assumptions on the constraint we can always prove weak convergence of the iterative scheme. In certain cases, i.e. for special families of convex constraints, weak convergence implies norm convergence. The presented approach covers a wide range of problems, e.g. Besov- or BV-restoration for which we present also numerical experiments in the context of image processing.

PDE methods for identifying ischemic heart disease. **Marius Lysaker** (Simula Research Laboratory, Norway), Bjørn Nielsen (Simula Research Laboratory, Norway) IC/MT3727/047

We explore the possibilities for using high speed laptops, mathematics and biological knowledge to construct a new medical imaging device. The source of the electrical potentials measured in ECG recordings at the body surface is the electrical pulses generated by the myocardium (heart). Our goal is to use ECG data and a geometrical model of the human body to compute an image of the potential distribution inside the heart wall. Since many heart conditions lead to changes in the potential pattern, such a device could be very useful for the physician.

Image inpainting and noise removal using the TV-Stokes equation. **Xue-Cheg Tai** (Universitetet i Bergen, Norway) IC/MT3438/047

In this talk, we propose a two-step algorithm for denoising digital images with additive noise and for inpainting of digital images. Observing that the isophote directions of an image correspond to an incompressible velocity field, we impose the constraint of zero divergence on the tangential field. Combined with an energy minimization problem corresponding to the smoothing of tangential vectors, this constraint gives rise to a nonlinear Stokes equation where the nonlinearity is in the viscosity function. Once the isophote directions are found, an image is reconstructed that fits those directions by solving another nonlinear partial differential equation. In both steps, we use finite difference schemes to solve. We present several numerical examples to show the effectiveness of our approach.

This talk is based on joint works with Stanley Osher and Talal Rahman.

IC/MP1/047: Non-standard and problem-oriented regularization methods.

Organiser: Sergei Pereverzyev (RICAM Linz, Austria)

Modern regularization theory has developed a general regularization scheme providing a uniform approach to the numerical treatment of ill-posed inverse problems. This general scheme includes such well-known regularization methods as Tikhonov and Lavrentiev regularization, Landweber iteration and others. At the same time, there exist regularization methods which use specific features of individual problems and, for this reason, can be applied only to them. The simplest example is a finite-difference scheme for numerical differentiation (classical ill-posed problem). Another important example is the quasi-reversibility method proposed by Lattes and Lions (1967) for solving the Cauchy problem for Laplace equation (one more classical ill-posed problem). Formally this method can be viewed as Tikhonov regularization, but a general theory cannot be used for its theoretical justification, because corresponding operator is unbounded. Other examples of methods falling into above mentioned category are the Method of lines proposed by Elden for the sideways heat equation, Local regularization methods for the solution of Volterra problems investigated by Lamm, Natural linearization method developed by Engl et al. for the parameter identification in nonlinear parabolic system, Regularization by Variance Components for geopotential determination from satellite data, and various forms of Regularization by discretization. Computational practice shows that such problem oriented methods are potentially very efficient, but they are not covered by a general theory and, as a result, some important questions related with their justification are still open. The goal of the Minisymposium is to bring together the experts, which have made recent contributions to the topic, with the aim to discuss a state of art and to elaborate a common platform for the development and implementation of Problem Oriented Regularization Methods.

Solving ill-posed Cauchy problems using regularization by discretization. **Lars Eldén** (Linköpings universitet, Sweden) IC/MT574/047

Sideways parabolic equations and the Cauchy problem for elliptic equations are examples of ill-posed Cauchy problems for PDE's. Such a problem can be written formally as an initial value problem

$$u_x = P(u), \qquad u(x_0) = u_0,$$

where the partial differential operator P is unbounded. Often the problem can be regularized by approximating the unbounded operator by a discretization, using e.g. wavelets or spectral methods. Stability results can be obtained.

We give a couple of examples of such problems, and describe how the discrete problems can be solved efficiently.

On the balancing principle for some problems of numerical analysis. **Shuai Lu** (RICAM Linz, Austria), Sergei Pereverzyev (RICAM Linz, Austria) IC/MT746/047

We discuss a choice of weight in penalization methods. The motivation for the use of penalization in computational mathematics is to improve the conditioning of the numerical solution. One example of such improvement is a regularization, where a penalization substitutes an ill-posed problem for a well-posed one. In modern numerical methods for PDEs a penalization is used, for example, to enforce a continuity of an approximate solution on non-matching grids. A choice of penalty weight should provide a balance between error components related with convergence and stability, which are usually unknown. In this paper we propose and analyze a simple adaptive strategy for the choice of penalty weight which does not rely on *a priori* estimates of above mentioned components. It is shown that under natural assumptions the accuracy provided by our adaptive strategy is worse only by a constant factor than one could achieve in the case of known stability and convergence rates. Finally, we successfully apply our strategy for self-regularization of Volterra-type severely ill-posed problems, such as the sideways heat equation, and for the choice of a weight in interior penalty discontinuous approximation on non-matching grids. Numerical experiments on a series of model problems support theoretical results. (Joint work with Prof. Raytcho D. Lazarov, Department of Mathematics, Texas A&M University)

The method of quasi-reversibility to solve the Cauchy problem for elliptic PDEs. **Laurent Bourgeois** (ENSTA, France), Eric Luneville (ENSTA, France) IC/MT951/047

This talk is devoted to the method of quasi-reversibility to solve ill-posed elliptic PDEs, which was first introduced in the late 60s by R. Lattès and J.-L. Lions. We first revisit the method in the general context of Tikhonov regularization of bounded or unbounded operators. Secondly, we apply the Morozov's discrepancy principle to it in order to make a relevant choice of the regularization parameter, and emphasize the interpretation of this choice in term of duality in optimization. Lastly, we show some numerical computations of the method of quasi-reversibility and of the associated Morozov's choice with the duality technique. These computations use nonconforming finite elements. Some error estimates are also presented.

Identification of parameters in nonlinear time-dependent PDEs via a multiharmonic ansatz. **Barbara Kaltenbacher** (Universität Stuttgart, Germany) IC/MT960/047

The problem of identifying coefficient functions in nonlinear time dependent PDEs from boundary measurements over some time interval, as arising e.g., in material characterization, is in practice often considered in frequency rather than in time domain. Here, it turns our that often a moderate number of higher harmonics suffices to describe the system with sufficient accuracy. Motivated by this fact, we propose a parameter identification method that is based on a multiharmonic expansion of the field quantities governed by the time dependent PDE under consideration. It turns out that an approximation of the coefficient function as a polynomial leads to a system of nonlinear but only space dependent PDEs. The (approximate) inverse problem then amounts to identifying polynomial coefficients appearing within this system, from additional boundary data. Regularization of the originally ill-posed problem of parameter identification is here achieved by finite dimensional projection (using the self-regularizing properties of discretization) as well as early stopping of the Newton iteration used for recovering the polynomial coefficients. In this talk we will explain the proposed method, provide some analysis and show numerical results.

IC/MP1/047: Non-standard and problem-oriented regularization methods. #2

Organiser: Sergei Pereverzyev (RICAM Linz, Austria)

(For abstract, see session #1 above.)

Regularization for gravitational-potential determination from space. **Juergen Kusche** (GFZ Potsdam, Germany), Jasper van Loon (TU Delft, The Netherlands) IC/MT978/047

The *decade of the geopotentials*, which had started with the launch of the CHAMP (Challenging Minisatellite Payload for Geophysical Application) satellite on July 15, 2000, has brought completely new data sets to the geodetic and geophysical communities, and initiated the development of new methodologies in the recovery of the Earth's gravitational and magnetic potentials from spaceborne measurements. Historically, the determination of the Earth's outer gravitational potential and the geoid - an equipotential surface coinciding with mean sea level - was undertaken from collecting huge quantities of surface, ship- and airborne gravity measurements by solving a free boundary-value problem, or alternatively from orbit perturbations of passive satellites or altimetric measurements of sea-surface heights. But with the CHAMP and successive GRACE spaceborne data sets we now have observations of unprecedented homogeneity and accuracy that allow today to determine and understand even the tiny temporal changes in the Earth's gravitational field caused by groundwater changes in larger reservoirs and non-steric sea-level variations.

Whereas the observation of the Earth's gravitational field from space has many advantages, it essentially poses an ill-posed problem because we need to perform downward continuation, because we have to deal with noisy discrete data of complicated correlation structure taken at different altitudes, and because of data gaps caused by insufficient satellite coverage. In geodesy, since the begin of the space age problem- oriented regularization methods have been developed: the expansion of the potential into truncated spherical harmonic series, the so-called Kaula method of regularization by introducing prior information, the collection of complementary data to fill data gaps, or the application of post-processing filter techniques to smooth the potentials. More recent studies have been looking into the applicability of Tikhonov-type and iterative regularization methods and parameter-choice strategies well-known in the inverse problems community, including regularization by estimating variance components, robust estimation methods,

and the construction of nonisotropic post-analysis filters. The talk will provide an overview on recent concepts and developments

On gradient methods for maximum entropy regularizing retrieval of atmospheric aerosol particle size distribution function. **Yanfei Wang** (Chinese Academy of Sciences) IC/MT987/047

The determination of the aerosol particle size distribution function using the particle spectrum extinction equation is an ill-posed integral equation of the first kind [1]. Even for finite moment case, the problem is still discrete ill-posed, since as is known, we are often faced with limited /insufficient observations in remote sensing and the observations are contaminated. To overcome the ill-posedness, regularization techniques are developed. However, most of the literature focuses on the application of Phillips-Twomey's regularization or its variants which is unstable in several cases. Recently in [2], the authors considered Tikhonov's smooth regularization method in $W^{1,2}$ space for ill-posed inversion. But the method still relies on the choice of the regularization parameter and the *a priori* estimation of the noise level. As is known, the particle size distribution is always positive and we are often faced with incomplete data. The concept of maximum entropy from information theory and statistic mechanics can be best used for this purpose. Therefore, in this paper, we study the maximum entropy based regularization method and develop a gradient method for solving the corresponding optimization problem. Our numerical tests are based on the remotely sensed data by CE 318 for Po Yang lake region of Jiang Xi Province which is a specified typical area by national 973 project, and are performed to show the efficiency and feasibility of the proposed algorithms.

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Local regularization for ill-posed Volterra inverse problems. **Patricia Lamm** (Michigan State University, USA) IC/MT1175/047

We will discuss recent developments in the theory and application of local regularization for ill-posed Volterra inverse problems. In particular, we will discuss extensions of the theory to allow for fast sequential solution of nonlinear equations as well as a discrepancy principle to select the size of the local regularization interval and qualitative properties of the measure used in the regularization process.

Landweber–Kaczmarz methods for regularizing systems of nonlinear ill-posed equations. **Antonio Leitao** (Universidade Federal de Santa Catarina, Brazil), Markus Haltmeier (Universität Innsbruck, Austria) IC/MT4281/047

In this talk we develop and analyze novel iterative regularization techniques for the solution of systems of nonlinear ill-posed operator equations. The basic idea consists in considering separately each equation of this system and incorporating a loping strategy. The first technique is a Landweber-Kaczmarz-type method, equipped with a novel stopping criteria. The second method is obtained using an embedding strategy, and again a Kaczmarz-type approach. We prove well-posedness, stability and convergence of both methods.

IC/MP147/047: Inverse and ill-posed problems in industry.

Organiser: Yanbo Wang (Fudan University, PR China)

This minisymposia is to bring together the people who are interested in the inverse and ill-posed problems in industry. The four speakers are experts in this field. They will present their new ideas and new results on this topic. The audiences can know the new development in this field. I think it will be very interesting for the audiences to have this chance to meet together in this minisymposia.

The impact of the noise-covariance structure upon the accuracy of indirect estimation. **Sergei Pereverzyev** (RICAM Linz, Austria) IC/MT425/047

The question addressed in the talk is: "How can colored observation noise be taken into account properly without direct access to a noise covariance operator?" Discussing inverse estimation from noisy observations it is reasonable to distinguish global and local regularization. Within a global regularization one tries to recover the whole solution as an element of some normed space. In local regularization the goal is to specify only some details such as a point value, or a wavelet/Fourier coefficient. We will show that in principle random colored noise allows us to obtain a better accuracy of a local regularization than deterministic noise.

For global regularization the situation is opposite: random colored noise will not *help* us to recover the whole solution. It gives a hint that optimal local regularization can be used as a *referee* for a global regularization in a sense that some global regularization strategy can be accepted if approximate solution, it provides, has point values or wavelet/Fourier coefficients which are close to ones estimated within the local regularization.

The talk is based on the results of a joint research with Frank Bauer and Peter Mathe.

How is a hidden rule found from operation data?. **Junichi Nakagawa** (Gakushuin University, Japan) IC/MT1799/047

Steel company researchers tend to focus on manufacturing processes. The phenomena are mostly complex, however, observations are limited because we must operate with high temperature objects and large-scale equipment. Consequently, we have been trying to find hidden rules from operation data. Supposed we show a map representing the position of these phenomena in four categories of the manufacturing process: stationary, non-stationary, linear and nonlinear, our phenomena fall into the non-stationary and nonlinear category. However, we donŠt have a general method by which this area can be analyzed. If mathematical principals can be applied in this area, we can have direct linkage between real phenomena and mathematics. Inverse problem is important to find hidden phenomena on manufacturing process from limited observation data. We show several examples of inverse analysis. These will enable reduced costs, and innovation in manufacturing processes.

A numerical method for solving the IHCP problem without initial value. **Yanbo Wang** (Fudan University, PR China) IC/MT2656/047

The inverse heat conduction problem (IHCP) arising in most thermal manufacturing processes of solids has recently attracted much attention. The typical case is the determination of the heat flux on an inaccessible boundary through measurements on an accessible boundary. In the real applications, only discrete data with noise at finite points are available for solving this problem . This problem is known to be extremely ill-posed. Here we will give a numerical method on how to reconstruct the heat flux without initial values. We will also discuss another problem of how to reconstruct the interval length by the measurement data at the boundary without initial values. Numerical examples show that our method is quite effective.

New approach for analytical solutions (by closed formulas) of non-linear direct and inverse problems for intensive steel quenching processes. **Sharif Guseynov** (Latvijas Universitate, Latvia) IC/MT4459/047

Intensive steel quenching (IQ) is one of effective contemporary methods for ecologically clean production of hard and superhard materials. The quality of article in the production process depends on various factors: critical heat fluxes, possible boiling process on the surface of hardware a.o. Some of these factors are difficult to measure experimentally and they must be estimated (calculated) theoretically.

In this paper, we mathematically describe IQ process by non-stationary heat equation (both - classical and hyperbolic) together with non-linear Newton type boundary condition (BC). We offer the new analytical method (by closed formulas) for the solutions of direct problems for both models of heat conduction process with above mentioned non-linear BC.

We solve the coefficient inverse problem for hyperbolic heat equation with non-linear BC in analytical form: we determine *relaxation time* parameter (coefficient at second time derivative in hyperbolic heat equation) assumed by the given temperature distribution at the end of production process.

We solve the initial inverse problem for the classical heat equation with the same non-linear BC: we reestablish the initial temperature distribution for infinite time interval without substantial additional information (we assume only the solution's boundedness).

IC/MP269/047: Inverse problems in financial modelling.

Organiser: Jorge Zubelli (Instituto Nacional de Matemática Pura e Aplicada, Brazil)
Co-organiser: Marco Avellaneda (Courant Institute, NYU, USA)
Co-organiser: Bernd Hofmann (TU Chemnitz, Germany)

The impact of advanced mathematical tools in financial engineering has been growing steadily during the past few decades. During the same period, the theory of inverse problems has been the subject of a lot of attention and has had tremendous impact in several applied fields ranging from medical imaging to geophysics. A number of crucial problems in finances can be cast as inverse problems. Model and volatility calibration is an example of one such problem. It is manifestly ill posed and calls for techniques from the inverse problem theory such as regularization as well as tools from statistics and optimization to handle the massive amount of noisy data.

In this mini-symposium we will present a panorama of practical as well as theoretical issues involved in financial modelling from the perspective of inverse problems. The main goal will be to give emphasis to applications of interest to the financial industry such as option and derivative pricing in different contexts and regimes. To accomplish that goal we will gather a diverse group of researchers some of them directly connected to the financial industry while others will bring in theoretical tools from regularization, asymptotic analysis, jump-diffusion processes and partial differential equations.

A probabilistic approach to inverse problems in option pricing. **Rama Cont** (Columbia University, USA) IC/MT2241/047

The inverse problem of recovering an option pricing model (or risk-neutral process) from a set of given market prices of options, known in finance as the *model calibration* problem, has been treated in the literature either as an exact inversion in presence of continuum data or by applying deterministic optimization methods to a (regularized) least squares formulation of it. These methods yield a single set of model parameters calibrated to market data and ignore the non-uniqueness of the solution, which reflects *model uncertainty*.

We propose a probabilistic approach to the model calibration problem, which takes into account the multiplicity of solutions: starting from a prior distribution on models and a set of observed option prices, we construct a random martingale measure, whose expectation yield an arbitrage-free pricing rule consistent with the observed option prices and whose dispersion properties can be used to quantify model uncertainty. We describe a Monte Carlo algorithm for computing prices under this rule and characterize the limit behavior of the algorithm, which is shown to possess a dual interpretation in terms of minimization of "model risk". This construction only involves a well-posed unconstrained minimization of a convex function, easily performed with gradient-based methods. This algorithm can be seen as a dynamic arbitrage-free version of Avellaneda et al.'s Weighted Monte Carlo algorithm applicable to a wide range of pricing models and products.

Our approach yields a non-trivial posterior distribution, instead of a single price, for exotic options and allows to simulate from this posterior distribution. As an example, we compute the posterior distribution for a barrier option given a set of European calls and puts, in a stochastic volatility model with jumps.

Identification of the speed function in a local Levy model for option pricing. **Heinz Engl** (RICAM Linz, Austria) IC/MT2138/047

Levy-models are a generalization of the well-known Black-Scholes model for option pricing where the asset prices are described by Levy-Processes. Within this class a special type - the so-called local Levy models - have been proposed (Carr et al.). Analogous to local volatility models they depend on an unknown function - the local speed function. We consider the calibration problem of local Levy models for European options, which can be formulated as a nonlinear inverse problem with the local speed function as unknown. This leads to a parameter identification problem in a parabolic partial integro-differential equation. We show that it can be solved in a stable way by nonlinear Tikhonov regularization and prove convergence and convergence rates for the regularized solutions under abstract smoothness conditions (so-called "source conditions"). Furthermore, these smoothness conditions indicate that this problem is more ill-posed than a similar local volatility calibration problem for the Black-Scholes model. Finally, we present the results of a numerical implementation of the regularization.

This work was done in collaboration with Hansjörg Albrecher (Graz Univ. of Tech./ RICAM Linz), Philipp Mayer (Graz Univ. of Tech.) and Stefan Kindermann (Ind. Math. Inst, University of Linz).

Estimating exponential Lévy models from option prices via Tikhonov regularization. **Moeiz Rouis** (École Polytechnique Palaiseau, France) IC/MT5026/047

In the class of exponential Lévy models [1], the dynamics of an asset is described by its diffusion coefficient $\sigma \geq 0$ and its Lévy measure ν, a positive (possibly infinite) measure on $R \setminus \{0\}$ verifying

$$\int \min(1, x^2)\nu(dx) < \infty, \qquad \int \nu(dx)e^x < \infty.$$

Option prices can then be shown to solve a partial integro-differential equation (PIDE) [2]. The model calibration problem in this context concerns the identification of the parameters (σ, ν) of the PIDE from a finite number of option prices. We propose a method which yields a stable solution for this *ill posed inverse* problem, using a Tikhonov regularization method plus a suitable parametrization of Lévy measure. We solve the resulting optimization problem by a gradient-based method where the gradient is computed by solving an adjoint PIDE with an explicit-implicit finite difference method [3]. We discuss theoretical aspects of the regularization procedure and test the performance of the algorithm on simulated data and market prices of options.

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Coefficient reconstruction in jump-diffusion models and interest rate modeling. **Cecilia Mancini** (Università di Firenze, Italy) IC/MT2964/047

We introduce a nonparametric technique to reconstruct the coefficients of a univariate jump-diffusion process when we have discrete time observations. The drift, diffusion and jump intensity functions are level dependent. The estimator of the diffusion coefficient is consistent even if the jump process has infinite activity. Our results rely on the fact that it is possible to disentangle the discontinuous part of the state variable through those squared increments between observations exceeding a suitable threshold. We apply our technique to re-examine the estimation of models for the short interest rate. With respect to alternative estimates, the proposed threshold technique provides narrower confidence intervals and, in some cases, very different results from those in the literature.

IC/MP269/047: Inverse problems in financial modelling. #2

Organiser: Jorge Zubelli (Instituto Nacional de Matemática Pura e Aplicada, Brazil)
Co-organiser: Marco Avellaneda (Courant Institute, NYU, USA)
Co-organiser: Bernd Hofmann (TU Chemnitz, Germany)

(For abstract, see session #1 above.)

Nature of ill-posedness and regularization of some benchmark problems in inverse option pricing. **Bernd Hofmann** (TU Chemnitz, Germany) IC/MT2315/047

Inverse problems in option pricing are frequently regarded as simple and resolved if a formula of Black-Scholes-type defines the forward operator. However, precisely because the structure of such problems is straightforward, they may serve as benchmark problems for studying the nature of ill-posedness occurring in the context of volatility calibration. In the first part of this talk, using a Hilbert space setting we analyze the inverse problem of calibrating a purely time-dependent volatility function from a term-structure of option prices by solving an ill-posed nonlinear operator equation in spaces of integrable functions over a finite interval. The smoothing forward operator of the inverse problem under consideration is decomposed into an inner compact linear convolution operator and an outer nonlinear Nemytskii operator determined by the Black-Scholes function. The nature of ill-posedness of the nonlinear composition problem is considered by means of the character of regularized solutions using Tikhonov's method. For the particular case of L^2, a detailed analysis of convergence rates is given, including the interpretation of the corresponding source conditions, which are related to multiplication operators. The second part of the talk is concerned with the singular case of at-the-money options, which plays an interesting role for the benchmark problem. For that case the Fréchet derivative of the forward operator degenerates. Consequently, the classical analysis of convergence rates established by Engl et al. 1989 cannot be applied directly. The talk presents an alternative approach based on Bregman distances bridging the gap between this singular case and the case of in-the-money and out-of-the-money options with respect to the benchmark problem. This is partially joint work with Torsten Hein (Chemnitz), Otmar Scherzer, Christiane Pöschl (Innsbruck) and Barbara Kaltenbacher (Stuttgart). Research is supported by DFG HO1454/7-1.

On maximum entropy regularization and descriptive regularization for parameter identification in a model with time-depending volatility. **Romy Krämer** (TU Chemnitz, Germany), Matthias Richter (TU Chemnitz, Germany) IC/MT2237/047

We consider two inverse problems of parameter identification in the generalized Black–Scholes model, where the asset price P_t at time t is described by

$$dP_t = \mu P_t\, dt + \sigma(t) P_t\, dW_t$$

with a time-dependent volatility fuction $\sigma(t)$ $(0 \leq t \leq T)$. As data we use maturity-dependent option prices $u(t)$ $(0 \leq t \leq T)$.

The first part of the talk is concerned with the inverse problem of identifying the squared volatility function $a(t) := \sigma^2(t)$ over the time interval $[0, T]$. By formulating this inverse problem as a nonlinear operator equation

$$F(a) = u \tag{1}$$

we discuss ill-posedness effects and the applicability of maximum entropy regularization, where the regularized solution a_α^δ is a minimizer of

$$\|F(a) - u^\delta\|^2 + \alpha \int_0^T a(\tau) \ln\left(\frac{a(\tau)}{\overline{a}(\tau)}\right) d\tau.$$

In this context u^δ denotes the noisy data and $\overline{a} \in L^\infty(0, T)$ a fixed reference function. We present results concerning convergence and convergence rates of the regularized solution

and compare the performance of maximum entropy regularization with Tikhonov regularization by means of a numerical case study.

The second part of the talk is devoted to the identification of the antiderivative

$$S(t) := \int_0^t \sigma^2(\tau)\, d\tau \quad (0 \le t \le T)\,.$$

As a motivation we point out that for pricing European call and put options (or more generally claims for which the final payoff depends only on the asset price at the maturity) the knowledge of S is sufficent. This inverse problem can be formulated as

$$N(S) = u\,, \tag{2}$$

where the forward operator N mapping in $C[0,T]$ is of Nemytzkii type. We classify the instabilities which occur in this situation as ill-conditioning effects and discuss the stabilizing effects of *a priori* information concerning the monotonicity of S.

On decoupling of volatility smile and term structure in inverse option pricing. **Torsten Hein** (TU Chemnitz, Germany) IC/MT2168/047

The identification of local volatility surfaces from market data of European Vanilla options is one very important example of inverse problem that arises in mathematical finance. As many other parameter identification problems, the reconstruction of local volatility surfaces is ill-posed, and reasonable results can only be achieved via regularization methods. Moreover, due to sparsity of data, the local volatility is not uniquely determined, but depends strongly on the kind of regularization norm used and a good a-priori guess for the parameter.

By assuming a multiplicative structure for the local volatility, which is motivated by the specific data situation, the inverse problem can be decomposed into two separate subproblems. This removes part of the non-uniqueness and allows to establish convergence and convergence rates under weak assumptions. Additionally, a numerical solution of the two subproblems is much cheaper than that of the overall identification problem.

The talk present joint work with Herbert Egger (Linz) and Bernd Hofmann (Chemnitz).

Inverse problems and regularization techniques in option pricing. **Jorge Zubelli** (Instituto Nacional de Matemática Pura e Aplicada, Brazil) IC/MT2552/047

In this talk we shall give an overview of a number of challenging mathematical problems that appear in the process of model calibration in financial applications related to option pricing. This will serve as a way of connecting many of the topics covered by the different speakers in the rest of the minisymposium.

A typical representative of the class of problems under consideration is that of determining the (local) volatility from quoted option prices. One usual approach to this problem is through Dupire's formula. At that point, we will also look at some directions for generalization of Dupire's formula for the local volatility in the case of baskets of options and several assets. This is joint work with P. de Napoli and P. Amster (UBA-AR).

Finally, we will discuss calibration of stochastic volatility models under different asymptotic regimes. This is joint work with M.O. de Souza (UFF-BR).

IC/MP509/015: Strongly-nonlinear phenomena: theory, integrability and applications to hydrodynamics, Bose–Einstein condensation and biology.

Organiser: Alejandro Aceves (University of New Mexico, USA)
Co-organiser: Tomáš Dohnal (ETH Zürich, Switzerland)
Co-organiser: Pavel Lushnikov (University of New Mexico, USA)

Numerous physical processes exhibit strong enough nonlinear effects to qualitatively alter the dynamics and produce phenomena that are completely foreign to linear dynamics. Examples of such systems relevant to this minisymposium include solitons or solitary waves in free surface hydrodynamics, internal waves, wave breaking in hydrodynamics, modulational instability, extreme waves in deep water, etc. A striking quality of some of the governing nonlinear partial differential equations is their complete integrability.

This minisymposium will address the latest results on mathematical modeling of the physical processes and analysis of the corresponding equations, their structure and solutions.

Transcitical flow over a step. **Roger Grimshaw** (Loughborough UNiversity, UK) IC/MT3708/015

In both the ocean and the atmosphere, the interaction of a density stratified flow with topography can generate large-amplitude, horizontally propagating internal solitary waves. Often these waves appear as a wave-train, or undular bore. In this talk we focus on the situation when the flow is critical, that is, the flow speed is close to that of a linear long wave mode. In the weakly nonlinear regime, this is modeled by the forced Korteweg de Vries equation. We will review how WhithamŠs modulation theory has been applied to obtain an analytical description of undular bores for flow over isolated obstacles, and then show how the same approach can be used for flow over a step.

Freak waves and dissipation due to wave-breaking. **Vladimir Zakharov** (University of Arizona, USA) IC/MT4850/015

Freak Waves add Dissipation due to Wave Breaking

Dispersive and non-classical shocks in the hyperbolic continuum-limit of FPU lattices. **Jens Rademacher** (CWI, Amsterdam, The Netherlands), Michael Herrmann (Humboldt-Universität zu Berlin, Germany) IC/MT3886/015

We consider the continuum limit of FPU chains (i.e., nearest neighbour coupled particles in a Newton potential) under hyperbolic scaling of particle index and time for shock-type Riemann problems. For the linear chain, Alexander Mielke has recently given a rather complete characterization in terms of Wigner measures for more general data. In particular, for oscillation free initial data, the limit is well described by the linear wave equation. In the nonlinear case, the description is much more delicate and is not contained in the naive limiting p-system of mass and momentum conservation. The measure valued limit still conserves mass, momentum and energy, which rules out Lax shocks. For the Toda potential and zero dispersion limits of some PDEs it is known that shocks are dispersive in nature. Recently, Whitham modulation equations of wave trains were formally deduced to describe the arising oscillations in more generality. We numerically confirm this ansatz and present evidence that for non-convex flux shocks can be undercompressive; i.e., non-classical. Such shocks are oscillation free and can be described by the underlying p-system.

Multi-dimensional compactons in nonlinear wave equations. **James Hyman** (Los Alamos National Laboratory, USA), Philip Rosenau (Tel Aviv University, Israel) IC/MT5055/015

Most solitions are one-dimensional waves, even in multidimensional equations. Solitons are nonlinear traveling waves where the nonlinearity and dispersion are balanced to create a stable coherent local environment so that that the solitions maintain their coherence when colliding with other solitions. Because the same dispersive operators are much stronger to two and three dimensions than in one dimension, this balance is usually lost when a one-dimensional equation is generalized to higher dimensions. We restore the balance by making the dispersion weaker in a class of KdV and regularized long wave equations to create fully two- and three-dimensional solutions.

IC/MP509/015: Strongly-nonlinear phenomena: theory, integrability and applications to hydrodynamics, Bose-Einstein condensation and biology. #2

Organiser: Pavel Lushnikov (University of New Mexico, USA)
Co-organiser: Tomáš Dohnal (ETH Zürich, Switzerland)

(For abstract, see session #1 above.)

Aggregation and critical collapse of bacterial colonies. **Pavel Lushnikov** (University of New Mexico, USA) IC/MT3593/015

Motion of bacteria can be described in microscopic limit through bacterial density. Bacteria secret chemical which attract other bacteria. Diffusion of emitted chemical provides highly nonlocal mechanism of attraction between bacteria. Nonlinear dynamics of bacterial colonies is described by Keller-Segel model which is dissipative but has many features which are strikingly reminiscent of nonlinear Schrödinger equation, including critical collapse in 2D and supercritical collapse in 3D. Typical evolution of 2D bacterial colonies in experiment is very slow (on scale of hours) until at some region of space the bacterial density exceeds critical value. After that bacterial colonies collapse on a scale of several minutes. Critical collapse of bacterial colonies has self-similar form with spatial scale $(t_0 - t)^{1/2}$, however, corrections to that law is not of loglog form, well known for nonlinear Schrödinger equation, but rather the exponent of the square root of logarithm of $(t_0 - t)$, which makes these corrections noticeable even for moderate bacterial densities. To prevent singularity of bacterial density, the finite size of bacteria should be taken into account. Large bacteria moves through random fluctuations of their membranes. The modified Keller-Segel equation is derived for the probability distribution function of membrane fluctuations which includes contact interaction between bacteria and prevents formation of singularities of bacterial density.

Stationary dispersive shock waves and oblique solitons in Bose-Einstein condensates. **Gennady El** (Loughborough University, UK), Arnaldo Gammal (Universidade de São Paulo, Brazil), Anatoly Kamchatnov (Russian Academy of Sciences) IC/MT3792/015

Recent experiments on expanding Bose-Einstein condensates (BEC) have revealed two types of patterns related to the formation of dispersive shock waves (DSW). One of them is connected with the breaking of the density profile in a freely expanding condensate and was studied by several authors both numerically and, in relevant approximations, analytically.
Another type of DSWs represents a counterpart of the stationary oblique compression jumps of traditional gas dynamics and is formed in the supersonic flow of a BEC past an obstacle. We develop a theory of such spatial DSWs in the frame of the time-independent, two-dimensional Gross-Pitaevskii equation. Corresponding analytical solutions for the asymptotic wave form of the DSW and for the accompanying linear "ship-wave" pattern before the obstacle are obtained and shown to be in excellent agreement with the density profiles in our full time-dependent numerical simulations. The possibility of observation of optical counterparts of the described multi-dimensional wave patterns in a BEC is discussed.

Localized modes in the nonlinear Schrödinger equation with periodic nonlinearity and periodic potential. **Vladimir Konotop** (Universidade de Lisboa, Portugal), Yuli Bludov (Universidade de Lisboa, Portugal) IC/MT3950/015

We consider spatially localized solutions of the nonlinear Schrödinger equation with periodic nonlinearity and periodic potential, concentrating on phenomena originated by competition between the two periodic terms. More specifically, we list physical problems governed by the model, describe numerical results on different branches of the solutions, discuss their stability and bifurcations, analyze asymptotic of the solutions near the different gap edges, and present lattice models generated by the Wannier function expansion of the original equation.

Interaction of two-colour spatial solitons in nematic liquid crystals. **Benjamin Skuse** (University of Edinburgh, UK) IC/MT4428/030

The interaction of two spatial solitary waves based on coherent light of two different wavelengths in a nematic liquid crystal (NLC) is investigated, such solitary waves being termed nematicons. In the local limit it will be shown that two colour nematicons are governed by a system of two saturable, coupled nonlinear Schrödinger (CNLS) equations. Approximate evolution equations for the beam parameters are derived using a hybrid variational technique which includes the effect of diffractive radiation shed as the beams propagate and interact. The approximate method will be presented briefly and solutions of the resulting approximate equations will be compared with numerical solutions of the full governing nematicon equations.

IC/MP508/015: Strongly-nonlinear phenomena in optical and/or periodic media.

Organiser: Tomáš Dohnal (ETH Zürich, Switzerland)
Co-organiser: Pavel Lushnikov (University of New Mexico, USA)

Numerous physical processes exhibit strong enough nonlinear effects to qualitatively alter the dynamics and produce phenomena that are completely foreign to linear dynamics. Examples of such structures relevant to this minisymposium include solitons or solitary waves in optical fibers and photonic crystals and catastrophic collapse and filamentation of laser pulses in many nonlinear media including atmosphere and plasma. These phenomena often cause strong dissipation or dispersion which prevents singular behavior such as classical shocks or blow-up.
This minisymposium will address the latest results on formulation of the corresponding mathematical models, their analysis and numerical approximations as well as on the relevant experimental achievements.

Time-domain simulations of nonlinear Maxwell's equations using Krylov-subspace methods. **Kurt Busch** (Universität Karlsruhe, Germany), Martin Pototschnig (Universität Karlsruhe, Germany), Jens Niegemann (Universität Karlsruhe, Germany), Lasha Tkeshelashvili (Universität Karlsruhe, Germany) IC/MT3717/015

Recent progress in micro- and nano-structuring of photonic materials with strongly nonlinear properties and/or embedded optically active elements such as quantum dots requires the quantitative modeling of ever more complex optical systems. In order to address this challenge, We propose a Krylov subspace based operator-exponential approach for solving nonlinear Maxwell's equations in the time domain. This approach exhibits significantly better performance than the standard Finite-Difference Time-Domain (FDTD) method as well as the classical Runge-Kutta scheme. In addition, our approach is flexible enough to incorporate various coupling effects of the electromagnetic fields with other physical systems and, therefore, is able to handle complex nonlinear problems.

Existence of (generalized) breathers in periodic media. **Guido Schneider** (Universität Stuttgart, Germany) IC/MT3865/015

Modulating pulse solutions consist of a pulse-like envelope advancing in the laboratory frame and modulating an underlying wave-train; they are also referred to as 'moving breathers' since they are time-periodic in a moving frame of reference. In this talk we discuss the existence of such solutions in periodic media using spatial dynamics and invariant manifold theory. Depending on the spectral gaps they can exist as breathers or generalized breathers, i.e. with small tails at infinity.

Gap solitons in a 2D periodic medium. **Dmitry Pelinovsky** (McMaster University, Canada) IC/MT3455/015

We address a two-dimensional nonlinear elliptic problem with a finite-amplitude periodic potential. For a class of separable potentials, we study bifurcation of the first band gap in the spectrum of the linear Schrödinger operator and the relevant coupled-mode equations to describe this bifurcation. We show analytically and numerically that the truncated coupled-mode equations admit a two-dimensional localized solution called a gap soliton. Persistence of the two-dimensional gap solitons of the coupled-mode equations in the full nonlinear elliptic problem is proved with rigorous analysis of Lyapunov–Schmidt reductions in the Fourier space.

Surface gap solitons at a nonlinearity interface. **Tomáš Dohnal** (ETH Zürich, Switzerland) IC/MT3830/015

We demonstrate existence of waves localized at the interface of two nonlinear periodic media with different coefficients of the cubic nonlinearity via the one-dimensional Gross–Pitaevsky equation. We call these waves the surface gap solitons (SGS).

In the case of smooth symmetric periodic potentials, we study analytically bifurcations of SGS's from standard gap solitons and determine numerically the maximal jump of the nonlinearity coefficient allowing for the SGS existence. We show that the maximal jump vanishes near the thresholds of bifurcations of gap solitons.

In the case of continuous potentials with a jump in the first derivative at the interface, we develop a homotopy method of continuation of SGS families from the solution obtained via gluing of parts of the standard gap solitons and study existence of SGS's in the photonic band gaps. We explain the termination of the SGS families in the interior points of the band gaps via the bifurcation of linear bound states in the continuous non-smooth potentials.

IC/MP508/015: Strongly-nonlinear phenomena in optical and/or periodic media. #2

Organiser: Stefano Trillo (Università degli Studi di Ferrara, Italy)
Co-organiser: Tomáš Dohnal (ETH Zürich, Switzerland)
Co-organiser: Pavel Lushnikov (University of New Mexico, USA)

(For abstract, see session #1 above.)

Intense optical pulses at UV wavelength. **Alejandro Aceves** (University of New Mexico, USA) IC/MT3633/015

To control and guide electrical discharges in air over distances of several meters a proposal is to ionize filaments of intense optical pulses, preferably at UV wavelength, combined with long infra-red pulses for plasma heating.

In this paper we study conditions of steady formation of pulse filaments coexisting with plasma formation. By numerical means, we derived stationary solutions of the governing nonlinear equations and discuss their stability. A goal of this project is to propose conditions on the plasma and features of the pulse for experimental realizations.

Nonlinear filamentation dynamics. **Daniele Faccio** (Università degli Studi dell'Insubria Como, Italy), Paolo Di Trapani (Università degli Studi dell'Insubria Como, Italy) IC/MT4847/015

We shall give an overview of ultra-short laser pulse filamentation dynamics as viewed within what we may call the X Wave model. Indeed, optical filamentation finds a particularly convenient description in terms of the spontaneous formation of stationary conical wave-packets in particular, in normal GVD, X Waves. We describe the experimental techniques implemented to analyze the strongly coupled space-time filament dynamics. Full angle-wavelength spectral analysis highlights the formation of conical emission, associated to X Wave formation, and axial supercontinuum, related to shock front formation. The spectra bear evidence of the well-known pulse splitting process associated to filamentation and that is here explained as the result of the spontaneous parametric generation and interaction of two X Waves that travel sub and super-luminally with respect to the input pump pulse. The interesting point is that while trailing shock fronts are expected as part of the filament dynamics and have been used to explain the blue shifted on-axis supercontinuum generation, measurements and numerics in condensed media clearly show evidence also of rising shock fronts within the same wave-packet. This finding, not explained by the standard approach to self-steepening and shock front formation, finds a natural explanation in the superluminal group velocity of the spontaneously formed X Waves. A brief overview will also be given of ongoing work on seeded filamentation: a weak seed pulse in the presence of an intense filament will undergo severe spatio-temporal reshaping mediated by cross-phase-modulation. This reshaping leads to the formation of an X Wave with a group velocity that is identical to that of the pump filament pulse. This opens the path for tunable generation of intense X Waves for applications.

Dynamics driven by dispersive shocks in the strong nonlinear regime of optics. **Stefano Trillo** (Università degli Studi di Ferrara, Italy), Claudio Conti (Università degli Studi di Roma "La Sapienza", Italy) IC/MT3725/015

We discuss the role of shock waves in recent nonlinear optics experiments conducted in the strongly nonlinear or weakly dispersive regime, and described by the integrable or nonintegrable (nonlocal) semiclassical Schrödinger equation with cubic potential. The hydrodynamic approximation of the starting model allows us to predict the formation of a single or multiple shock waves. We find, however, that the post-shock evolution is regularized by the occurence of fast oscillations caused by dispersive (in the temporal case) or diffractive (in the spatial case) effects, which leads to non-dissipative (collisionless) shocks. In four-wave mixing experiments driven by two interfering laser beams in a defocusing medium, the oscillations take the form of dark soliton channels. The output pattern is determined by collisions of solitons from adjacent periods, and the phenomenon is described in the framework of the scattering transform on the periodic line. In the context of spatial experiments, i.e. diffraction of a single bell shaped beam, it is important to investigate the role of nonlocality which, having a potential averaging effect, could hamper the formation of the shock. Conversely we find that the shock is robust against nonlocality, though the latter can alter the scenario and the output pattern. Moreover an analytic approach valid in the strong nonlocal limit suggests that the shock has impact also on the dynamics in the focusing regime.

Discrete cavity solitons. **Falk Lederer** (Universität Jena, Germany), Oleg Egorov (Universität Jena, Germany) IC/MT3893/015

Discrete systems, such as semiconductor superlattices, molecular chains, waveguides arrays, or coupled pendulums, share many interesting and somehow intriguing features. Following the theoretical predictions the existence of discrete solitons have been experimentally verified in waveguide arrays, being a prominent example for a discrete system, with either cubic or quadratic nonlinearity. Light propagation in such arrays exhibits striking anomalies in comparison with beams propagating in usual continuous systems, such as *discrete diffraction*, which can be controlled in size and sign by the input conditions. Consequently, solitary waves are likewise expected to behave differently in discrete systems. A logical step is to extend these studies towards dissipative systems (nonlinear waveguide array with dielectric mirrors at the end faces: Fabry–Perot cavity) where gain and losses play a significant role. Over the years a bundle of nonlinear effects has been studied in 1D (film) and 2D (bulk) Fabry–Perot cavities (continuous system) where canonical diffraction occurs. The interplay of feedback, loss, gain and nonlinearity leads to a considerably richer dynamical behavior than that observed in conservative systems. The system can adapt to the driving field in different ways, giving rise to multistability, and, as consequences, pattern formation, and other types of spatial self-organization. In particular, so-called cavity solitons (CS) may exist on a stable and preferably flat background. They represent localized defects and can either locally increase (bright CSs) or decrease (dark CSs) the transmission of the Fabry–Perot cavity. Once excited by a local change of the incident field, in principle, they stay forever on a flat holding beam, even if the initial excitation has been switched off. It is only natural to extend these studies towards discrete systems. Recently, the existence and properties of discrete cavity solitons were firstly studied in an array of coupled waveguide cavities endowed with Kerr nonlinearity. These studies have been extended towards quadratic nonlinearities. In the present contribution we discuss the existence, properties, and interactions of various types of discrete cavity solitons exploiting the control of the linear diffraction properties.

IC/MP417/015: Boundary-value problems and integral equations.

Organiser: Pavel Krutitskii (Keldysh Institute of Applied Mathematics RAS, Russian Federation)

The aim of this session is to screen recent developments in boundary value problems and relative theory of integral equation. The emphasis will be given to constructive methods, which either enable us to obtain integral representation for a solution or enable us to study its qualitative properties. Appropriate integral representation can be used in numerical analysis of the problems and in asymptotic analysis. Special attention to be given to theory of singular integral equations which occur in boundary value problems. It is expected that talks will cover the following topics: qualitative methods for boundary value problems, boundary value problems in cracked domains, integral equation methods in scattering theory and in potential theory, boundary value problems for Stokes equations, methods of functional analysis in boundary value problems, elliptic problems in nonsmooth domains, applications of integral equation methods in fluid dynamics; local and asymptotic methods in boundary value problems.

Helmholtz equation in domains bounded by closed curves and open arcs. **Pavel Krutitskii** (Keldysh Institute of Applied Mathematics RAS, Russian Federation) IC/MT474/015

Boundary value problems in planar domains bounded by closed curves and open arcs were not actively treated before though they have many applications. Similar domains model cracked solid bodies or they model several obstacles and screens in a fluid. However problems in domains bounded by closed curves and problems in the exterior of open arcs were treated separately, because different methods were used in their analysis. Problems for the Helmholtz equation in domains bounded by closed curves are reduced to the Fredholm equation of the 2-nd kind in text books on PDEs. Problems in the exterior of open arcs in a plane were reduced by single and double layer potentials to an equation of the 1-st kind with either logarithmic or strong singularity in the kernel (logarithmic for Dirichlet problem, while strong fot Neumann problem). If we combine these two methods for domains bounded by closed curves and open arcs, we obtain integral equation of different type and with different singularities at different parts on the boundary. The analysis of this equation is too complicated. In the present talk we reduce the Dirichlet and Neumann problems for Helmholtz equation in arbitrary domains bounded by closed curves and open arcs to the uniquely solvable Fredholm integro-algebraic equations of the 2-nd kind and index zero by a boundary integral equation approach. So, the classical result known for domains bounded by closed curves is extended to domains with closed and open boundary. Dirichlet and Neumann problems for the propagative Helmholtz equation are studied for exterior domain, while problems for dissipative Helmholtz equation are studied in both interior and exterior domains. Our method enables us to prove well-posedness of each problem (i.e. existence of the unique classical solution) and to obtain integral representation for a solution in the form of potentials.

A boundary-value problem for an infinite elastic strip with a semi-infinite crack. **Hiromichi Itou** (Gunma University, Japan) IC/MT3422/049

In this talk we consider a boundary value problem for an infinite elastic strip with a semi-infinite crack. The mass forces are supposed to be zero; on the crack the free traction boundary conditions are posed. The usage of the plane elastic single and double layer potentials reduces the problem to a system of singular integral equations. It is shown that this system is uniquely solvable in the appropriate Hölder spaces by the Fredholm alternative. This research is a joint project with Prof. Tani of Keio University.

Asymptotic behaviour of solutions of some nonlinear parabolic and elliptic equations with nonlinear boundary conditions. **Vladimir Kondratyev** (Moscow State University, Russian Federation) IC/MT3316/049

Let Ω be a bounded domain in $\mathbf{R^n}$ with a Lipshitz boundary $\partial\Omega$ and L be a symmetric elliptic operator in divergence form:

$$Lu \equiv \sum_{i,j} \frac{\partial}{\partial x_i} a_{i,j}(x) \frac{\partial u}{\partial x_j}$$

where the coefficients a_{ij} are bounded and measurable in Ω. We study the properties of solutions to equation

$$\frac{\partial u}{\partial t} - Lu + f(x,u) = 0 \text{ in } \Omega \times (0,\infty),$$

satisfying to nonlinear boundary value condition

$$\frac{\partial u}{\partial \nu} + g(x,u) = 0,$$

where ν is conormal vector.

Assume $f(x,u)$, $g(x,u)$ satysfy the following conditions:

$$f(x,0) = g(x,0) = f_u(x,0) = g_u(x,0) = 0, \quad f_u(x,u) > 0,\ g_u(x,u) > 0 \text{ for } u \neq$$

We show that any positive solution vanishing at ∞ is asymptotically equivalent as $t \to \infty$ to a solution of non-linear ordinary differential equation of first order

$$\dot{\alpha} = -\frac{\int_\Omega f(x,u)dx + \int_{\partial\Omega} g(x,u)ds_x}{mes\,\Omega}, \quad \alpha(0) = 1.$$

We also study the elliptic problem:

$$\frac{\partial^2 u}{\partial t^2} + Lu - f(x,u) = 0.$$

Theory of generalized J-integral. **Kohji Ohtsuka** (Hiroshima Kokusai Gakuin University, Japan) IC/MT3292/049

Generalized J-integral (abbr. GJ-integral) is proposed in 1981 to describe three-dimensional fracture phenomena. In 1985, GJ-integral is extended to be applicable to various elliptic boundary value problems. Main property of GJ-integral is to catch the singularity of weak solutions in boundary value problems, which is described as follows: Let Ω be a bounded domain in R^N, $f \in L^2(\Omega)^m$ a given function with a integer $m \geq 1$ and $V(\Omega)$ a subspace of $H^1(\Omega)^m$. Find $u \in V(\Omega) \subset H^1(\Omega)^m$ minimizing the potential energy functional $\mathcal{E}(v,\Omega)$. For u, GJ-integral $J_\omega(u,X) = P_\omega(u,X) + R_\omega(u,X)$ is defined as the functional with two parameters an open set ω and a vector field X. Let us say that u is regular in ω, if $u|_{\omega\cap\Omega} \in H^2(\Omega \cap \omega)^m$. If u is regular in ω, then $J_\omega(u,X) = 0$ for all $X \in W^{1,\infty}(\overline{\omega})^N$. Now consider the perturbation $\{\Omega(t)\}_{0\leq t\leq T}$ of the domain Ω and the variational problems finding the minimizer $u(t)$. The main theorem in GJ-integral theory is:

$$\left.\frac{d\mathcal{E}(u(t),\Omega(t))}{dt}\right|_{t=0} = -R_\Omega(u,X) + \int_\Omega \{X \cdot \nabla(f \cdot u) + (f \cdot u)\mathrm{div}\, X\}\, dx$$

Starting from the main theorem, we can derive results on shape sensitivity analysis using the zero property for regularity.

IC/MP417/015: Boundary-value problems and integral equations. #2

Organiser: Pavel Krutitskii (Keldysh Institute of Applied Mathematics RAS, Russian Federation)

(For abstract, see session #1 above.)

Boundary integral equations and maximum-modulus estimates for the Stokes system. **Werner Varnhorn** (Universität Kassel, Germany) IC/MT1588/015

In the theory of partial differential equations the classical maximum principle is well-known. It states that any non-constant harmonic function u takes its maximum (and minimum) values always at the boundary ∂G of the corresponding domain G. For higher order differential equations as well as for systems of differential equations such a principle does not hold in general. In these cases, however, there is some hope for a so-called maximum modulus estimate of the form

$$\max_G |u(x)| \ \leq\ c \max_{\partial G} |u(x)|, \qquad (1)$$

where c denotes some constant. We prove the validity of an estimate (1) for the linear Stokes system

$$-\Delta u + \nabla p = 0 \quad \text{in } G, \quad \nabla \cdot u = 0 \quad \text{in } G, \quad u = b \quad \text{on } \partial G$$

concerning the unknown velocity vector u and an unknown pressure function p of a viscous incompressible fluid flow via the method of boundary integral equations. Here $G \subset \mathbb{R}^n$ $(n \geq 2)$ is some bounded or unbounded open set having a compact boundary ∂G of class $C^{1,\alpha}$ $(0 < \alpha \leq 1)$.

Boundary-integral method for Stokes flow past porous bodies. **Mirela Kohr** (Universitatea Babeş-Bolyai, Romania) IC/MT2936/049

In this talk we present a new indirect boundary integral method in order to study the Stokes flow of an unbounded viscous incompressible fluid past a porous body of arbitrary shape. The flow inside the porous body is described by the Brinkman model. Asymptotic results related to the force on the porous body are also obtained in both case of large and also low permeability. Several applications and other connected results will be presented.

Quadrature formulas for the periodic functions for solutions to boundary value problems for the Laplace equation. **Alexander Petrov** (Moscow State University, Russian Federation) IC/MT3281/049

We consider boundary value problems for the Laplace equation in planar and axially symmetric domains. Problems are reduced to the Fredholm equation with logarithmic singularity. We discuss quadrature formulas for a certain integral. The integrand in this integral is a periodic function with logarithmic singularity. We obtain a quadrature formula for this integral in case of an even number N of markers at the boundary line. Formula is accurate for all trigonometric polynomials of order N. We obtain the approximation of the Fredholm equation by a system of linear algebraic equations with the high accuracy. The accuracy of the method checked for different hydrodynamics problems: potential flow over many bodies, cavity flow, breaking capillary-gravity waves, Rayleigh-Taylor instability, fluid fluctuation in vessels, cumulative jets forming, inner waves between two flows.

IC/MP1094/025: Analysis and numerical issues in kinetic equations.

Organiser: Jennifer Proft (University of Texas at Austin, USA)
Co-organiser: Irene Gamba (University of Texas at Austin, USA)
Co-organiser: Maria Gualdani (University of Texas at Austin, USA)

To discuss the state of the art, specifically, analytical and computational issues of classical and semi-classical kinetic transport theory and those related to evolution of probability measures. Such issues will involve non-conservative phenomena associated with Boltzmann, Wigner, and Fokker–Planck type equations, their long time dynamics, non-equilibrium states, approximating properties, and numerical discretizations. Discussion of comparisons of deterministic versus stochastic computational schemes.

WENO solvers for the Boltzmann–Poisson system for semiconductor devices. **María Cáceres** (Universidad de Granada, Spain) IC/MT2453/049

Statistical models are used to describe electron transport in semiconductors at a mesoscopic level. The basic model is given by the Boltzmann transport equation for semiconductors in the semi-classical approximation coupled with Poisson's equation, since the electric field is self-consistent due to the electrostatics produced by the electrons and the dopants in the semiconductor.
In this talk we show WENO-solvers for this system for different devices, for the 1-dimensional and 2-dimensional cases. The main differences of the devices are in the material (Si or GaAs) and the geometries (MOSFET or MESFET).
The deterministic numerical scheme is based on WENO finite differences for the advection part and a Runge-Kutta scheme for the evolution in time, after considering the change of variables proposed by Fatemi and Odeh in the parabolic band approximation case and later extended by Majorana and Pidatella for the non-parabolic approximation case (Kane model).

Analysis for the 1-dimensional case for Si were given by Carrillo-Gamba-Majorana-Shu who later extended it for the 2-dimensional case for MESFET devices. The 1-dimensional case for GaAs was studied by Carrillo, Majorana and the author.

Results for the double-gate MOSFETs, where there are two bands of oxide will be presented.

The discontinuous Galerkin method for semiconductor Boltzmann–Poisson system. **Armando Majorana** (Università degli Studi di Catania, Italy), Irene Gamba (University of Texas at Austin, USA), Jennifer Proft (University of Texas at Austin, USA) IC/MT2625/049

The simulation of semiconductor devices has become a standard tool in the construction process. A very detailed description of the transport processes in semiconductors is provided by kinetic transport models. The semi-classical Boltzmann equation coupled with the Poisson equation provides a general theoretical framework for modeling electron transport. Moreover, time-dependent solutions of the Boltzmann equation contain all the information on the evolution of the carrier distribution. Very recently, deterministic solvers to the Boltzmann-Poisson system for two-dimensional devices were proposed. These methods provide accurate results which agree well with those obtained from Monte Carlo simulations. However, a large number of grid points (a few million) is required, when treating two-dimensional problems. This implies a great amount of CPU time for each simulation. In this paper, we propose a new way of discretizing the Boltzmann-Poisson system based on the discontinuous Galerkin method. This allows the use of a not uniform grid and reduces the CPU time. We show the results of some simulations and the comparisons with solutions obtained using WENO scheme.

Stochastic dynamics of long supply chains with random breakdowns. **Christian Ringhofer** (Arizona State University, USA) IC/MT3040/049

We analyze the stochastic large time behavior of long supply chains via a traffic-flow type random particle model. So items travel on a virtual road from one production stage to the next. Random breakdowns of the processors at each stage are modeled via a Markov process. The result is a conservation law for the expectation of the part density which holds on time scales which are large compared to the mean up and down times of the processors.

Scaling dynamics of Smoluchowski's coagulation equations with dust and gel. **Robert Pego** (Carnegie Mellon University, USA) IC/MT3397/049

We study limiting behavior of rescaled size distributions that evolve by Smoluchowski's rate equations for coagulation, with rate kernel $K = 2$, $x + y$ or xy. We find that the dynamics naturally extend to probability distributions on the half-line with zero and infinity appended, representing populations of clusters of zero and infinite size. The "scaling attractor" (set of subsequential limits) is compact and has a Levy-Khintchine-type representation that linearizes the dynamics and allows one to establish several signatures of chaos. In particular, for any given solution trajectory, there is a dense family of initial distributions (with the same initial tail) that yield scaling trajectories that shadow the given one for all time.

IC/MP1094/025: Analysis and numerical issues in kinetic equations. #2

Organiser: Jennifer Proft (University of Texas at Austin, USA)
Co-organiser: Irene Gamba (University of Texas at Austin, USA)
Co-organiser: Maria Gualdani (University of Texas at Austin, USA)

(For abstract, see session #1 above.)

On the blowing-up of solutions to quantum hydrodynamic equations in bounded domains. **Maria Gualdani** (University of Texas at Austin, USA) IC/MT3791/049

The blow-up in finite time for the solutions to the multi-dimensional quantum hydrodynamic model in a bounded domain is proved. The model consists on conservation of mass equation and a momentum balanced equation equivalent to a compressible Euler equations corrected by a dispersion term of the third order in the momentum balance. The proof is based on a-priori estimates for the energy functional for a new observable constructed with an auxiliary function, and it is shown that under suitable assumptions on the initial and boundary data the solution blows up after a finite time.

Semiconductor energy-transport equations and beyond. **Jüngel Ansgar** (TU Wien, Austria) IC/MT4245/049

Parasitic effects in modern semiconductor devices with characteristic lengths of less than 70 nanometer are becoming more and more significant in industrial applications, making necessary an accurate modeling of the physical phenomena. In this talk we will concentrate on thermal effects in semiconductors, modeled by energy-transport equations. These equations can be derived in the diffusion limit from the semiconductor Boltzmann equation using an entropy maximization precedure. The resulting model consists of nonlinear cross-diffusion parabolic equations for the electron density, electron energy density, and electric potential. The equations are discretized employing exponentially fitted mixed finite elements and modern MOS transistors are simulated in two and three space dimensions. Moreover, it will be explained how a complete hierarchy of diffusive higher-order moment equations can be derived from kinetic models, extending the energy-transport model.

Self-similarity for granular gases of inelastic hard spheres. **Clément Mouhot** (Université de Paris–Dauphine, France) IC/MT4392/049

Discontinuous Galerkin approximation of the linear Boltzmann transport equation. **Jennifer Proft** (University of Texas at Austin, USA), Irene Gamba (University of Texas at Austin, USA) IC/MT3786/049

We analyze the problem of numerically solving linear variants of the space inhomogeneous multidimensional linear Boltzmann equation under the action of electrostatic potentials. We develop a discontinuous Galerkin positive preserving discretization and show, based on discrete entropy multipliers, that the discrete method produces a monotone, stable, converging scheme. By using the decaying estimate to statistical equilibrium solutions, we are able to control the domain of definition of the scheme, uniformly in time, and consequently obtain stable error estimates in W^{k+1} spaces. In generaly, deterministic methods can be very accurate for problems in which the solution may or may not be far from thermodynamical equilibrium and high accuracy is required. Additionally, they yield specific details of transient solutions and consequently can be more efficient than the traditional probabilistic Monte Carlo techniques for the computation of transients. Theoretical and numerical results of our scheme are presented.

04: Partial Differential Equations, Contributed Talks

IC/CTS4601/04: **Regularity theory, well-posedness.**

Organiser: Goro Akagi (Shibaura Institute of Technology, Japan)

On mathematical and physical correctness of balance equations for atmospheric dynamics. **Andrei Bourchtein** (Universidade Federal de Pelotas, Brazil), Ludmila Bourchtein (Universidade Federal de Pelotas, Brazil) IC/CT651/042

The partial differential equations of atmospheric dynamics represent a complex system with multiple space and time scales. The time spectrum of actual large scale motions contains as the principal component the slow synoptic processes with characteristic period of one-two days, while faster waves have quite small amplitudes. However, the solutions to the atmosphere dynamics equations are very sensitive to the type of initial values and small perturbations to actual atmospheric fields can generate the fast gravity waves of great amplitude, which are not observed in the real atmosphere.

Contemporary atmosphere forecasting and modeling consists of numerical solution of the governing partial differential equations. The initial conditions supplied by data assimilation schemes are slightly different from actual atmospheric fields. Therefore some restrictions onto initial values should be imposed in order to avoid physically unrealizable oscillations. These restrictions usually form a set of nonlinear stationary partial differential equations (so-called balance equations) to be solved by appropriate numerical method. It is well known that iterative methods of solution diverge for some physically natural types of balance equations, but the cause of this behavior was not clear. The speculations about the reasons of the divergence were centered on two possibilities: shortcomings of the iterative algorithms or ill-posedness of the boundary value problems. In this study, using concept of ellipticity in the sense of Douglis-Nirenberg, we show that boundary value problems for some types of balance equations can be ill-posed, which reflects in divergence of the iterative methods of solution. We also consider some examples of the real atmosphere circulations when ellipticity conditions are not satisfied.

Coefficients of the singularities for elliptic boundary-value problems in polygonal and polyhedral domains. **Boniface Nkemzi** (University of Buea, Cameroon) IC/CT698/042

Solutions of elliptic boundary value problems in domains with corners or edges are known to have singular behaviours even when the data of the underlying problem are very smooth. These singularities affect the accuracy of the finite element method throughout the whole domain. Thus, it is necessary to develop adaptations which improve the accuracy of the finite element approximations.

Using asymptotic methods, it has been shown that the solution u of an elliptic boundary value problem with corner or edge singularities can be broken down into the sum

$$u = w + \lambda S$$

of a regular part w, whose behavior is not affected by the presence of the corners or edges, and a singular part λS, where S is an explicitly known singular solution.

In the numerical solution of such a problem the regular part w is well approximated by the usual finite element methods. Up till date calculating accurately the coefficient (stress intensity factor) λ remains a very serious problem, especially in three dimensions. As such the theoretical results have had very little practical implications.

In this presentation, we consider boundary value problems for the Laplace equations in polygonal and polyhedral domains and derive explicit expressions for the computations of the coefficients of the corner and edge singularities.

Doubly-nonlinear evolution equations with non-monotone perturbations. **Goro Akagi** (Shibaura Institute of Technology, Japan) IC/CT1187/033

The existence of strong solutions to Cauchy problems for doubly nonlinear abstract evolution equations with non-monotone perturbations in reflexive Banach spaces is proved under appropriate assumptions, which allow the case where solutions of the corresponding unperturbed problem may not be unique. To prove the existence, a couple of approximate problems are introduced and delicate limiting procedures are discussed by using various tools from convex analysis and the Schawder-Tychonoff fixed point theorem. Furthermore, applications of abstract evolution equations to nonlinear PDEs are also given.

Coupled system of Korteweg–de Vries equation-type in domains with moving boundaries. **Octavio Vera** (Universidad del Bío-Bío, Chile), Mauricio Sepúlveda (Universidad de Concepción, Chile), Vanilde Bisognin (Universidad Franciscana, Brazil) IC/CT4577/042

We consider the initial-boundary value problem in a bounded domain with moving boundaries and nonhomogeneous boundary conditions for the coupled system of equations of Korteweg - de Vries type. We prove a global existence and uniqueness for strong solutions for the coupled system of equations of Korteweg - de Vries type as well as the exponential decay of small solutions in asymptotically cylindrical domains. Finally, we present a numerical scheme based in semi-implicit finite differences and we give some examples to show the numerical effect of the moving boundaries for this kind of systems.

Function-theoretic approach to anisotropic plane elasticity. **Alexander Soldatov** (Belgorod State Univesity, Russian Federation) IC/CT4728/042

The representation of general solutions of Lamé system of plane elasticity is given with the help of so-called Douglis analytic functions. Using integral representation of these functions the basic boundary value problems for Lamé system are reduced to equivalent singular integral equations on the boundary.

IC/CTS4605/04: Iterative methods, functional differential equations.

Organiser: Juergen Geiser (Humboldt-Universität zu Berlin, Germany)

Seismic sources and waves using iterative operator splitting methods. **Juergen Geiser** (Humboldt-Universität zu Berlin, Germany) IC/CT2880/025

We discuss iterative operator splitting method for wave-equations motivated from a realistic problem in seismic sources and waves. The operator-splitting methods are welknow to solve such complicated multidimensional and multi physics problems. We present an idea for the consistency analysis of the underlying iterative methods as theoretical background. The mathematical methods are analytical sin and cos semi-groups, which represent the solution of a second order ODE. We discuss stable spatial discretization methods for the wave-equation with respect to the boundary conditions. We verify our methods for test problems with known analytical solutions. Multi-dimensional examples in seismic problems are done with the proposed methods. Finally we discuss the results with standard methods.

Tensor-product methods for stochastic problems. **Elmar Zander** (TU Braunschweig, Germany), Hermann Matthies (TU Braunschweig, Germany) IC/CT2414/004

In the solution of stochastic partial differential equations (SPDEs) the in general already huge dimension N of the algebraic system resulting from the spatial part of the problem is blown up by the huge number of degrees of freedom P coming from the stochastic part. The number of degrees of freedom of the complete system will be NP, which poses severe demands on memory and processor time. We will present a way of how to approximate the system by a tensor product (using its Karhunen-Loève decomposition with M terms), which uses only memory in the order of $M(P+N)$, and keeping this representation also inside the iterative linear solvers. Comparisons with full solvers will be given concerning memory and processor time as well as errror estimates and convergence results.

On an abstract Euler–Poisson–Darboux type equations. **Assia Guezane Lakoud** (Annaba University, Algeria), Chaoui Abderrezak (Skikda University, Algeria) IC/CT410/043

In this talk we study a Cauchy boundary value problem generated by Euler–Poisson–Darboux type equations with operator coefficients possessing variable domains. This work has been motivated by a series of recent results on a similar family of problems without singularity, we can mention the works in [2,3]. Under certain conditions on the operator coefficients, in a Hilbert space, we show that the problem is well posed in the Hadamard sense. The proofs rely on a generalization of the well known energy method. First, we derive *a priori* estimates for strong solutions with the help of Yosida operator approximation. Then, using previous results, we show that the range of the operators of our problem is dense.

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On the matrices with operator entries. **Djurdjica Takači** (Univerzitet u Novum Sadu, Yugoslavia) IC/CT760/043

In this paper we consider the matrices with Mikusiński operator entries. We construct a method for determining an approximate solution of the matrix equations, which enables calculations with numbers instead of operators. The analysis of the existence of a solution and its character, is done by using the nonsingularity results related to real or complex numbers.

Existence and uniqueness of solution to a nonlinear dead-oil model resulting from oil engineering. **Moulay Rchid Sidi Ammi** (University Of Aveiro, Department of Mathematics„ Portugal) IC/CT800/043

In this paper we study a *dead-oil* isotherm system resulting from classical modelings of oil engineering. We prove the existence of solution using time discretization. The uniqueness is established in a particular class of admissible solutions.

On the approach to the gelation phase of an aerosol. **Hans Babovsky** (TU Ilmenau, Germany) IC/CT4464/044

Gelation is a phase transition at which coagulating aerosol particles (mathematically described by the Smoluchowski equation) cluster to macroparticles. The understanding and numerical simulation of this phenomenon is of high interest in a number of applications.

Particularly interesting is the situation of a coagulating system in a diffusive random environment. Analytic investigations show that stochastic effects eventually turn a stable situation into a metastable one which finally ends up with gelation [1].

Recently, numerical schemes have been proposed for the efficient simulation of the transition to the gel phase [1,2]. This is at present applied to back up and visualize theoretical results and to proceed into domains presently not available to theory.

In the talk, recent analytical and numerical results are presented.

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IC/CTS4617/04: .

Organiser: Angela Jimenez-Casas (Universidad Pontificia Comillas, Spain)

Some results on coupled linear wave equations. **Saadet Erbay** (Isik Üniversitesi, Turkey), Alp Eden (Bogazici University, Turkey), Irma Hacinliyan (Istanbul Technical University, Turkey) IC/CT2327/015

We obtain integral representation of solution to the following coupled linear wave equations

$$\begin{aligned} \phi_{1,xx} - \phi_{1,yy} - \beta\phi_{2,xy} &= f, \\ \phi_{2,xx} - \lambda\phi_{2,yy} - \beta\phi_{1,xy} &= g, \end{aligned} \qquad (1)$$

where $f, g \in L^1(\mathbb{R}^2) \bigcap C(\mathbb{R}^2)$. These equations are the real components of a system that is called a generalized Davey-Stewartson system consisting of a nonlinear Schrödinger type equation for the complex amplitude of a short wave coupled with two linear wave equations for long waves propagating in an infinite elastic medium. This asymmetrically coupled system cannot be decoupled. So we write the system as a first order linear system in terms of characteristics and solve it directly. A representation of solution of the non-homogeneous system is given by

$$\phi_1(x,y) = \int_{\mathbb{R}^2} [K_1(x',y',x,y)\, f(x',y') + K_2(x',y',x,y)\, g(x',y')]\, dx'dy$$

$$\phi_2(x,y) = \int_{\mathbb{R}^2} [K_2(x',y',x,y)\, f(x',y') + K_3(x',y',x,y)\, g(x',y')]\, dx'dy$$

where the kernel functions $K_i(x',y',x,y)$, $(i = 1,2,3)$ are products of Heaviside functions that live on different characteristic lines. Using these integral representations we find upper bounds for the L^∞ norms of solutions as well as the energy of the system.

Quaternionic analysis and applications. **Dimitrios Pinotsis** (University of Reading, UK) IC/CT4545/015

We present two novel applications of the theory of Quaternions: (a) The solution of certain boundary value problems for linear elliptic Partial Differential Equations (PDEs) in four dimensions. (b) The explicit computation of certain three dimensional integrals without integrating with respect to the real variables. Both applications are based on an important formalism in complex analysis, the so called Dbar formalism, and its quaternionic generalizations. The relevant results have been published in [1], [2].

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Asymptotic behavior for a general phase-field model with more than two phases. **Angela Jimenez-Casas** (Universidad Pontificia Comillas, Spain) IC/CT4396/015

We consider a generalization of the semilinear phase field model from [1], by using a more general density function which describe the phase separation of mixtures of three or more components, instead of binary mixtures. The main objective of this work is to prove the existence of metastable solutions that evolve very slowly in time, for this general model.

Next, we show several numerically experiments to obtain these metastable patterns in bough cases, for the model with two different phases and for more of two different phases.

Finally we consider a general enthalpy function which allows to study more general couplings between a diffusion field and a phase-field. For instance, the phase field can be seen as the density of bacterial collony or the mass of growing tumor. Analogously, the diffusion field can stand for the density of nutrient. In this case we prove also the existence of the metastable solutions of the generalized system.

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Convergence to equilibrium for nonlinear evolution equations. **Hao Wu** (Fudan University, PR China) IC/CT4889/000

In this talk we will present the Łojasiewicz–Simon approach for the study on convergence of global solution to equilibrium for some nonlinear evolution equations subject to dissipative boundary condition. Those nonlinear evolution equations include:

(1) the Cahn–Hilliard equation with dynamical boundary condition;
(2) the damped semilinear wave equation with critical exponent and dissipative boundary condition;
(3) the parabolic–hyperbolic phase-field system with dissipative boundary condition.

The work was done in collaboration with Prof. Maurizio Grasselli and Prof. Songmu Zheng respectively.

Diffraction of light. **Matthias Kunik** (Universität Magdeburg, Germany) IC/CT640/015

The diffraction of light is considered for a plane screen with an open infinite slit by solving the Maxwell-Helmholtz system in the upper half space with the Fourier method. The corresponding solution is given explicitely in terms of the Fourier-transformed distributional boundary fields. The method deals with all components of the electromagnetic field and leads to a modification of Sommerfeld's scalar diffraction theory. Using this approach we can represent each vectorial solution satisfying an appropriate energy condition by its boundary fields in the Sobolev spaces $H^{\pm 1/2}$. This representation includes also solutions with smooth boundary fields, which are not covered by Sommerfeld's solutions of boundary integral equations (or integro-differential equations) with Hankel kernels. On the other hand we show that Sommerfeld's theory using a boundary integral equation for the so called B-polarisation leads in general to vectorial solutions which violate a necessary energy condition. For the physically admissible regular solutions in the upper half space we derive the necessary and sufficient energy conditions in terms of the Fourier transformed distributional boundary fields.

On the asymptotic behavior of the Korteweg–de Vries equation with localized damping. **Ademir Pazoto** (Universidade Federal do Rio de Janeiro, Brazil) IC/CT1881/015

The purpose of this work is to study the exponential stabilization of the Korteweg-de Vries equation posed in the right half-line, as well as, in a bounded domain, under the effect of a localized damping term. Combining multiplier techniques and compactness arguments the problem is reduced to prove the unique continuation property of weak solutions. Here, the unique continuation is obtained in two steps: we first prove that solutions vanishing on any subinterval are necessarily smooth and then we apply the unique continuation results available in the literature. In particular, we show that the exponential rate of decay is uniform in bounded sets of initial data. Similar conclusions remain valid for the critical generalized Korteweg-de Vries equation.

IC/CTS4593/04: Miscellaneous computation.

Linear stability analysis of infiltration fronts for a non-equilibrium Richards equation. **Carlota Cuesta** (University of Nottingham, UK) IC/CT4722/015

Gravity-driven fingers in unsaturated porous media flow have been observed experimentally by a number of researchers. It is known that the standard Richards equation does not suffice to describe instability during infiltration processes. In recent years extensions of the Richards equation have been considered in order to pursue fingering. Among these extensions, an equation containing a third order term with mixed derivatives has been also postulated. This includes the so-called non-equilibrium Richards equation, which results from considering a *dynamic* capillary pressure relation, as suggested by Hassanizadeh and Gray (1993). In this talk we recall our results on existence of travelling waves solutions of the latter. We concentrate in a field soil model for which the diffusivity can be regarded constant. We shall first present an analysis of linear stability of travelling waves in one dimension, and later recall the long-wave stability criterion in higher dimensions. Instabilities are confirmed by means of numerical computations in two dimensions. We shall finally derive and analyse the non-linear evolution equation of the fingers at the instability onset. This equation turns out to be a forward-backward pseudo-parabolic equation.

Systems of multi-dimensional singular integral equations in non-smooth domains: a Noetherian property and index. **Vladimir Vasilyev** (Bryansk State University, Russian Federation) IC/CT3346/015

On manifolds with non-smooth boundaries the Mikhlin–Calderon–Zygmund type operators with a matrix symbol are considered. The singularities of a boundary can be consisting of cones and wedges sheaf. The Noetherian property conditions (wave factorization) and reduction to Atiyah–Singer theorem are described.

These results were obtained through joint work with I.V. Scherbenko.

Variant H-measures and applications. **Martin Lazar** (University of Zagreb, Croatia), Nenad Antonić (University of Zagreb, Croatia) IC/CT1862/015

H-measures have been introduced as a tool for studying quadratic terms of weakly converging L^2 sequences. As such, they have proved appropriate for exploring limits of energy terms. Due to special scaling of the dual variable $(\frac{\xi}{|\xi|})$ included in the definition of H-measures, they have mostly been used for hyperbolic equations and systems. The above scaling turned out to be unsuitable for the applications to equations of parabolic type. Therefore, a variant of H-measures has been developed, containing a different scaling for the dual variable, which is better suited to the equations of this type.

I shall present the construction of the new variant, and its properties. Applications to the heat and Schrödinger equation will be compared with the results obtained by the original H-measures, where the results turned out to be insufficient, as the corresponding H-measures are supported in two points (North/South pole) of the dual space. The new variant gives measures supported on the curves, thus enabling a study of propagation phenomena. The explicit relations between macroscopic energy dissipation term and source term are obtained, as well. Furthermore, application to the non-stationary Stokes system allows us to express the term which appears by homogenisation via the variant H-measure.

Existence of solutions for some quasi-linear elliptic systems with measure data. **Zakaria El Allali** (Université Mohammed Premier Oujda, Morocco), Abdelaziz Chetouani (Université Mohammed 1er Oujda, Morocco), Najib Tsouli (Université Mohammed Premier Oujda, Morocco), El Bekkaye Mermri (Université Mohammed Premier Oujda, Morocco) IC/CT636/015

We are concerned here with the existence of solutions for quasi-linear elliptic systems such as:

$$\begin{aligned} -\Delta u &= au + bv + f_1(x,u,v,\nabla u,\nabla v) + \mu_1 \ \text{ in } \Omega,\\ -\Delta v &= bu + dv + f_2(x,u,v,\nabla u,\nabla v) + \mu_2 \ \text{ in } \Omega,\\ u &= v = 0 \ \text{ on } \partial\Omega, \end{aligned}$$

where Ω is a bounded open set in $\mathbb{R}^N$, $N \geq 2$, $1 < p < +\infty$, a, b, d are given real numbers $\mu_i (i = 1, 2)$ is a Radon measure on Ω and $f_1, f_2 : \Omega \times \mathbb{R} \times \mathbb{R}^N \to \mathbb{R}$ are assumed to be Carathéodory functions. We will prove the existence of a solution $(u, v) \in (H_0^1(\Omega))^2$, if and only if the signed measure $\mu_i (i = 1, 2)$ is zero on sets of capacity zero in Ω; i.e $\mu_i(E) = 0$ $(i = 1, 2)$ for every set E such that $\mathrm{cap}_p(E, \Omega) = 0$.

Stable combined compact-difference scheme with an arbitrary boundary condition. **Kazuya Matsuoka** (Nagoya University, Japan) IC/CT4378/038

Direct numerical simulations of the flows with various physical phenomena such as turbulent flows and/or flows generating aeroacoustic noise require high-resolution numerical methods. Recently, implicit finite difference schemes such as the Padé scheme are studied as the high resolution finite difference schemes. One example is a spectral-like Compact Difference (sp-CD) scheme proposed by Lele. However, in order to improve the accuracy of CD scheme, many stencils must be used. Therefore, the treatment of CD scheme at the points near the boundary is different from that at the inner points. Carpenter and Kobayashi shows that the treatment of boundary in CD schemes for the spatial derivatives is important for the stability of time marching equations. Higher derivatives on 3 stencils are used in Combined Compact Difference (CCD) schemes proposed by Chu&Fan and Nihei&Ishii. Using CCD scheme, we can obtain higher accuracy and higher resolution of at the points near the boundary except for the boundary point. However, the stability analysis of CCD schemes is not studied in detail. In this study, we investigate 1) the stability of CCD scheme, 2) a more stable CCD scheme on non-periodic boundary condition and 3) a new scheme for the regular grid system in which the boundary is allocated between regular grid points. The fully discrete equation for 1-D advection-diffusion equations are investigated, in which CCD scheme is used for spatial derivatives and the Runge-Kutta (RK) method is used for the time marching with various Courant number and diffu-

sion number. The stability region was given for periodic and non-periodic boundary conditions. We proposed a new CCD scheme for non-periodic boundary conditions with larger stable region than that for periodic boundary conditions. We also proposed an extended stable scheme for the regular grid system in which the boundary is allocated between regular grid points.

Some types of stability estimates for operator-differential equations and operator-difference schemes. **Boško Jovanović** (University of Belgrade, Yugoslavia) IC/CT675/015

An abstract problem $Au = \varphi$ is called stable if its solution u continuously depends on the input data φ. For linear problems this is equivalent to *a priori* estimate

$$\|u\|_1 \le \varrho \, \|\varphi\|_2$$

where $\|\cdot\|_1$ and $\|\cdot\|_2$ are certain norms. For evolution problems the quantity ϱ in many cases depends on the time variable t. In particular, the behavior of $\varrho(t)$ when $t \to +\infty$ is of interest. If ϱ does not depends on t the problem is called globally stable. If $\varrho(t) \to 0$ when $t \to +\infty$ the problem is called asymptotically stable.

Another type of stability is the strong stability, or the stability of the solution u under perturbations of operator A. Let $\tilde{u}$ be the solution of equation with perturbed operator $\tilde{A}\tilde{u} = \varphi$. A priori estimate of the strong stability have the form

$$\|\tilde{u} - u\|_3 \le \varrho \, \|\tilde{A} - A\|_4 .$$

In this case the problem is nonlinear, even for linear A and $\tilde{A}$, and the quantity ϱ depend on u and $\tilde{u}$. In the case of differential equations operator A is generally unbounded and one must have a suitable definition of its norm.

Present paper deals with the construction of different types of stability estimates for operator-differential equations and operator-difference schemes.

IC/CTS4595/04: Reaction-diffusion equations, steady-state solutions, bifurcation.

Organiser: Peter Pang (National University of Singapore)

New theory of spatio-temporal chaos in nonlinear systems of partial differential equations. **Nikolai Magnitskii** (Institute for Systems Analysis RAS, Russian Federation) IC/CT4164/040

During several last years, it was proved by author and his pupils that there exists one universal scenario of transition to dynamical chaos in nonlinear dissipative systems of ordinary differential equations, including all classical chaotic systems such as Lorenz, Rossler, Chua systems, Duffing-Holmes and generalized Matie equations and others (see [1] and references there). This scenario begins with the Feigenbaum cascade of period doubling bifurcations of stable cycles, continues by the Sharkovskii subharmonic cascade of bifurcations of stable cycles with arbitrary periods and then continues by the Magnitskii homoclinic cascade of bifurcations of stable cycles convergent to homoclinic contours. In the present talk we consider three systems of partial differential equations: the system of Brusselator equations as an example of a reaction - diffusion system, the Kuramoto-Tsuzuki (Time-Dependent Ginzburg-Landau equation) and the Magnitskii system of market economy equations. We show that at least one universal scenario realizes in all these systems. It is the subharmonic cascade of bifurcations of two-dimensional tori along one or both frequencies. This cascade also can be described by the universal Feigenbaum-Sharkovskii-Magnitskii (FSM) theory. In conclusion we show that the following conjecture is likely to be true: the appearance of spatio-temporal chaos in nonlinear systems of partial differential equations is caused by cascades of bifurcations of two-dimensional invariant tori rather than the destruction of a three-dimensional torus with the generation of some hypothetical strange attractor, as it is assumed in modern publications following the Ruelle-Takens paper [2].

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Energy estimates for reaction–diffusion processes of electrically charged species. **Annegret Glitzky** (Weierstraß-Institut Berlin, Germany) IC/CT1313/040

We describe the transport of m different charged species in heterostructures via the processes drift, diffusion and reversible reactions of mass action type. The model contains continuity equations for the densities of all involved species which are coupled with a Poisson equation for the self-consistent calculation of the electrostatic potential which causes the drift of the charged particles. Forced by applications from semiconductor technology, we formulate rather general assumptions concerning the state equations, $u_i = u_i^* g_i(v_i)$, $i = 1, \dots, m$, relating the density u_i and the chemical potential v_i, such that Boltzmann and Fermi-Dirac statistics are included as special cases. Here u_i^* is some reference density depending on the position because of doping or heterogeneous materials. The free energy has the form

$$F = \sum_{i=1}^{m} F_i + F_{el}, \quad F_i(u_i) = \int_\Omega u_i^* \int_{g_i(0)}^{u_i/u_i^*} g_i^{-1}(z) \, \mathrm{d}z \, \mathrm{d}x,$$

where F_{el} denotes the electrostatic part of the free energy. The anti-gradient of the electrochemical potential ζ_i is supposed to be the driving force for the mass flux j_i,

$$j_i = -u_i^* g_i'(v_i) S_i(\cdot) \nabla \zeta_i, \quad i = 1, \dots, m,$$

where the matrix function S_i prescribes the possible anisotropy of the material. Additionally, the inverse Hessian of $F_i(u_i)$ has to be a factor in the flux term for the i-th species. The problem is completed by initial conditions and boundary conditions, which are compatible with thermodynamic equilibrium.

On solutions of the model equations the free energy decays monotonously and exponentially to its equilibrium value. The delicate step in the proof of the exponential decay of the free energy is an estimate of the free energy by the dissipation rate which can be proved indirectly. Moreover, we present energy estimates for related discretized problems.

A positive and conservative second-order finite-volume scheme. **Philipp Andrea Zardo** (Universität Kassel, Germany), Andreas Meister (Universität Kassel, Germany), Joachim Benz (Universität Kassel, Germany) IC/CT2214/040

The longterm development of water quality in rivers and canals strongly depends on phosphorus in both water and sediment as well as on the interaction of phosphorus with algae and zooplankton. Modelling leads to a system of stiff hyperbolic/parabolic partial differential equations. Additionally the crucial *positivity* property of all biological and chemical values and the *conservativity* property concerning the chemical constituents are to be fulfilled by the scheme, to obtain reasonable results.

In this talk a second order (in space and time) finite volume scheme which improves the time integration by weighting the

sink and source terms will be presented. The new scheme extends the modified Patankar-Ansatz by applying the approach also to sink terms and corresponding source terms of all non-conservative and positive constituents. Thus it guarantees the *positivity* similarly for these values, obtains *conservativity* for all *conservative* items and allows equal or larger timesteps Δt than the straight forward use of the underlying CFD-scheme.

Numerical results will be analysed to confirm the theoretical propositions.

Fractional diffusion equation and diffusive stresses. **Yuriy Povstenko** (Jan Dlugosz University, Poland) IC/CT774/040

The classical theory of difusion is based on the Fick law relating the matter flux vector to the concentration gradient. In combination with the balance equation for mass, this equation leads to the parabolic diffusion equation. The time-nonlocal dependence between the flux vector and corresponding gradient with long-tale power kernel can be interpreted in terms of fractional integrals and derivatives and yields the time-fractional diffusion equation. A quasi-static uncoupled theory of diffusive stresses based on this equation was introduced in [1,2]. In the present contribution several problems are solved in the framework of the proposed theory.

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Existence and uniqueness for a class of stochastic partial differential equations with application in tumor growth. **Fejzi Kolaneci** (University of New York, Tirana, Albania) IC/CT421/040

We consider the martingale problem associated with a quasilinear stochastic partial differential equation driven by a space-time white noise. Under suitable assumptions, the existence of weak solutions is proved via Girsanov's theorem, by an approximation procedure, and by a tightness argument. Using a moment duality method we investigate the uniqueness in law of the weak solution. The obtained theoretical results are applied to model the tumor growth for dispersed cells regime in the presence of adjuvant chemotherapy, immunotherapy, or gene therapy.

Stationary patterns in diffusive predator–prey models. **Peter Pang** (National University of Singapore) IC/CT4586/040

In this talk, we will describe some recently studied predator–prey models involving diffusion and cross-diffusion. In particular, we will describe our results concerning the existence of stationary patterns. In some of these cases, we find that certain stationary patterns arise only with the presence of cross-diffusion. This illustrates clearly the role played by cross-diffusion in complex population dynamics, such as when the species exercise defensive strategies or when stage structures are present.

IC/CTS4596/04: Reaction-diffusion equations, steady-state solutions, bifurcation.

Organiser: Lourdes Tello (Universidad Politécnica de Madrid, Spain)
Co-organiser: Juan Francisco Padial (Universidad Politécnica de Madrid, Spain)

Constructing exact solutions of reaction–diffusion–convection equations arising in mathematical biology. **Roman Cherniha** (National Academy of Sciences of Ukraine, Kyiv), Olexii Pliukhin (National Academy of Sciences of Ukraine, Kyiv) IC/CT3055/040

The nonlinear reaction–diffusion–convection (RDC) equation is:

$$u_t = (u^m u_x)_x + \lambda u^n u_x + C(u),$$

where $u = u(t,x)$ is the unknown function, $C(u)$ is an arbitrary smooth function and the subscripts t and x denote differentiation with respect to these variables, n, m and λ are some parameters. This kind of equation generalizes a great number of the known nonlinear equations describing various processes in biology; see, e.g.,[1]. While there is no existing general theory for analytical integrating nonlinear RDC equations of the above form, construction of particular exact solutions for these equations is a non-trivial and important problem. Now the most powerful methods for construction of exact solutions to nonlinear RDC equations are the group-theoretical approaches, which are based on using the Lie and conditional symmetries of a given equation.

In this talk, a complete description of conditional symmetries of the RDC equation is presented[2,3]. Furthermore those symmetries are applied for finding exact solutions of some RDC equations arising in mathematical biology. The exact solutions obtained are also applied for solving nonlinear boundary-value problems, with basic equations of the above form and zero Neumann conditions, and compared with the relevant numerical solutions obtained by a numerical technique[4].

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A complete classification of bifurcation diagrams of a p-Laplacian Dirichlet problem. **Shin-Hwa Wang** (National Tsing Hua University, Taiwan) IC/CT1236/004

We study the bifurcation diagrams of classical positive solutions u with $\|u\|_\infty \in (0,\infty)$ of the p-Laplacian Dirichlet problem

$$(\varphi_p(u'(x)))' + \lambda f_{q,r}(u(x)) = 0, \quad \text{for } -1 < x < 1, \text{ with } u(-1) = u(1) = 0,$$

where $p > 1$, $\varphi_p(y) = |y|^{p-2}y$, $(\varphi_p(u'))'$ is the one-dimensional p-Laplacian, $\lambda > 0$ is a bifurcation parameter, and

$$f_{q,r}(u) = \begin{cases} |1-u|^q, & \text{for } 0 < u \le 1, \\ |1-u|^r, & \text{for } u > 1, \end{cases}$$

with positive constants q and r. We give explicit formulas of bifurcation curves of classical positive solutions on the $(\lambda, \|u\|_\infty)$-plane. More importantly, for different (p,q,r), we give a complete classification of all bifurcation diagrams. Hence we are able to determine the (exact) multiplicity of classical positive solutions for each (p,q,r,λ).

A complete classification of bifurcation diagrams of classes of p-Laplacian multiparameter boundary value problems. **Kuo-Chih Hung** (National Tsing Hua University, Taiwan), Shin-Hwa Wang (National Tsing Hua University, Taiwan) IC/CT1240/040

We study the bifurcation diagrams of positive solutions of the p-Laplacian multiparameter boundary value problem

$$(\varphi_p(u'(x)))' + f_{\lambda,\mu}(u(x)) = 0,$$

for $-1 < x < 1$, with $u(-1) = u(1) = 0$, where $p > 1$, $\varphi_p(y) = |y|^{p-2}y$, $(\varphi_p(u'))'$ is the one-dimensional p-Laplacian, and $f_{\lambda,\mu}(u) = g(u,\lambda) + h(u,\mu)$, $\lambda > \lambda_0$, $\mu > \mu_0$ are two bifurcation parameters. We assume that functions g and h satisfy hypotheses ((H1)–(H3) and (H4a)) or ((H1)–(H3) and (H4b)). Under these hypotheses, we give a complete classification of bifurcation diagrams, and we prove that, on the $(\lambda, \|u\|_\infty)$-plane or $(\mu, \|u\|_\infty)$-plane, each bifurcation diagram consists of exactly one curve which is either a monotone curve or has exactly one turning point where the curve turns to the right. Hence the problem has at most two positive solutions for each $\lambda > \lambda_0$ and $\mu > \mu_0$. More precisely, we prove the exact multiplicity of positive solutions. In addition, for $p = 2$ or $p \geq 3$, we give interesting examples which show complete evolution of bifurcation diagrams, as μ or λ varies.

Bifurcation of positive solutions to Hénon equation. **Zhong-hua Yang** (Shanghai Normal University, PR China), Zhao-xiang Li (Shanghai Normal University, PR China) IC/CT1255/040

The boundary value problem of the Hénon equation $g(u,r) = \Delta u + |x - x^0|^r |u|^{q-1}u = 0$ with $x \in \Omega$ and $u|_\Gamma = 0$, is considered, where Δ is Laplace operator, $r \geq 0$, $x = (x_1, x_2)$, $x^0 = (\frac{1}{2}, \frac{1}{2})$, Ω is the unit square, and Γ is the boundary of Ω. The bifurcation method is applied to solving the D_4-symmetric positive solutions of the Hénon equation. Taking r as a bifurcation parameter, the $D_4 - \Sigma_d(D_4 - \Sigma_1, D_4 - \Sigma_2)$ symmetry-breaking bifurcation point is found on the branch of the D_4-symmetric positive solutions of the Hénon equation via the extended system. Finally, $\Sigma_d(\Sigma_1, \Sigma_2)$-symmetric solutions are computed by the branch-switching method based on the Liapunov–Schmidt reduction.

Stability in anomalous reaction–diffusion systems. **Yana Nec** (Technion – Israel Institute of Technology), Alexander Nepomnyashchy (Technion – Israel Institute of Technology) IC/CT84/010

Diffusion is a ubiquitous process, encountered in physics, chemistry and biology. Normal diffusion, i.e. unrestricted random walk, is often not a satisfactory model. For instance, diffusion in gels (especially bio-gels), porous media and polymers is slower than normal. On the other hand, the transport in plasma or turbulent flows is enhanced. Pattern formation in such anomalous systems, governed by integro-differential equations, is still hardly investigated. In this contribution we focus on two most non-trivial cases: (i) Turing instability in sub-diffusive systems; (ii) longwave oscillatory instability in super-diffusive systems.

We first treat the case of equal anomaly exponents of the reacting components. We find that the wave number range of monotonously growing disturbances is semi-infinite and is shifted into the short wave region when the diffusion coefficients' ratio approaches its critical value. There are two unstable modes per wave number in that range. For longer waves an oscillatory mode is present, unstable even when the coefficients' ratio exceeds its critical value for the monotonous modes. An exact formula is derived for the critical value of the coefficients' ratio, corresponding to the threshold of oscillatory instability in a sub-diffusive system.

In the case of distinct anomaly exponents, we show that when the exponents' difference is in favour of the inhibitor (activator) and of unity order, the system is unstable (stable). When the exponents' difference is small, an intermediate range of unstable wave numbers, dependent on the diffusion coefficients' ratio, is observed.

Also, we consider the case of a long wave oscillatory instability in a super-diffusive system. It is shown that near the instability threshold the problem is governed by a super-diffusive modification of the complex Ginzburg-Landau equations. We investigate the modulational instability of homogeneous oscillations and traveling waves, and discuss its nonlinear development.

Stationary solutions to a climate model with a nonlinear diffusive boundary condition. **Lourdes Tello** (Universidad Politécnica de Madrid, Spain) IC/CT4326/040

We study a model based in one proposed by R.G. Watts and R. Morantine ("Rapid climatic change and the deep ocean", Climatic Change 16, (1990) pp.83–97) modelling the temperature coupling surface deep ocean. The model consists of an equation of parabolic type for the temperature in a global ocean with a dynamic and diffusive nonlinear boundary condition. The boundary condition is obtained through a averaged global energy balance for the atmosphere surface temperature.

We prove that the number of stationary solutions depends on a parameter Q, which appears in the boundary condition modelling the amplitude of the source term induced by the superficial co-albedo.

This is a work in collaboration with J.I. Diaz (Univ. Complutense de Madrid).

IC/CTS4598/04: Asymptotic solutions, asymptotic domain decomposition.

Organiser: Kersten Schmidt (ETH Zürich, Switzerland)
Co-organiser: Anne-Laure Dalibard (Université de Paris–Dauphine, France)

Homogenization of scalar conservation laws with vanishing viscosity. **Anne-Laure Dalibard** (Université de Paris–Dauphine, France) IC/CT4324/041

We study the behavior as $\varepsilon \to 0$ of the solutions of the equation

$$\partial_t u^\varepsilon + \mathrm{div}_x \left[A\left(\frac{x}{\varepsilon}, u^\varepsilon\right)\right] - \varepsilon \Delta_x u^\varepsilon = 0, \quad t > 0,\ x \in \mathbb{R}^N,$$
$$u^\varepsilon(t=0,x) = u_0\left(x, \frac{x}{\varepsilon}\right)$$

where A is a given nonlinear flux, periodic with respect to its first variable. The homogenized problem can be computed by means of formal two-scale expansions.

When the initial data is already adapted to the micro-structure, the function u^ε behaves in L^1_{loc} as $v(x/\varepsilon, \bar{u}(t,x))$ as $\varepsilon \to 0$, where v is determined by a cell problem and $\bar{u}$ is the solution of the homogenized problem. The proof relies on the use of a kinetic formulation adapted to the parabolic conservation law.

When the initial data is not well-prepared, there is an initial layer during which the solution adapts itself to match the profile dictated by the environment. The typical size of the initial layer is of order ε. The proof relies strongly on the parabolic form of the equation; in particular, no condition of nonlinearity on A is required.

We also tackle the associated hyperbolic problem, i.e. the homogenization of equation $\partial_t u^\varepsilon + \mathrm{div}_x [A(x/\varepsilon, u^\varepsilon)] = 0$. We prove that a strong convergence result holds, even though the identification of the asymptotic profile is in general an open problem.

Approximation of highly conductive thin sheets with asymptotic expansion. **Kersten Schmidt** (ETH Zürich, Switzerland), Sébastien Tordeux (INSA Toulouse, France) IC/CT3101/041

Sensitive measurement and control equipment is protected from disturbing electromagnetic fields by thin shielding sheets[3]. Alternatively to discretisation of the sheets, the electromagnetic fields are modeled only in the surrounding of the layer taking them into account with the so called Impedance Boundary Conditions (IBCs) [4,2].

We study the shielding effect by means of the model problem of a diffusion equation with additional dissipation in the curved thin sheet. We use asymptotic expansion techniques [1] to derive a limiting problem (namely, as the thickness of the sheet ε tends to zero), as well as modelling contributions to the solution of higher orders in ε. These problems are posed in the limiting regime of vanishing ε, with a condition for a jump in the solution and it's normal derivative. This avoids having to use a mesh for the computational domain, even just locally, at the scale of ε.

We derive the problems for arbitrary order and show their existence and uniqueness. Numerical experiments for the problems up to second order show the asymptotic convergence of the solution to appropriate order in the thickness parameter ε.

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Method of multiple scales with three time scales. **Peter Kramer** (Rensselaer Polytechnic Institute, USA), Adnan Khan (Rensselaer Polytechnic Institute, USA), Robert DeVille (Courant Institute, NYU, USA), Philip Stathos (Rensselaer Polytechnic Institute, USA) IC/CT3539/041

Some confusion appears in the literature regarding the extension of the method of multiple scales to three or more time scales. While the work of Murdock and Wang correctly indicate some obstructions to such an extension in some types of problems, other work suggests that the extension should almost never be possible. These pessimistic results generally follow from the imposition of additional restrictions in the calculation, which really are not necessary. We will show on some simple ODE models how a systematic implementation of the method of multiple scales can succeed in correctly capturing three active time scales, though more calculation is required than one might expect from naive considerations. On the other hand, an extension of the method of averaging to three time scales produces an incorrect approximation in these problems. We will also discuss the method of multiple scales to two PDE systems with three time scales: one involving transport by a periodic velocity field with a strong mean flow and one involving the stochastic dynamics of a particle in a metastable potential.

A new shallow water model, by asymptotic analysis, with linear dependence on depth. **Raquel Taboada-Vázquez** (Universidade da Coruña, Spain), Jose Manuel Rodriguez Seijo (Universidade da Coruña, Spain) IC/CT1570/041

In this paper, we study the Euler equations in a domain with small depth. With this aim, we introduce a small adimensional parameter ε related to the depth and we use asymptotic analysis to study what happens when ε becomes small.

Usually, when used asymptotics to analyze fluids, they are used in the original domain (see[2]), that in this case depends on parameter ε and time t^{ε}, or the surface is supposed to be constant. We, however, shall use the asymptotic technique in the same way as in [1] and related works, that is, we do a change of variable to a reference domain independent of the parameter ε and the time.

In this way we obtain a model for ε small that, after coming back to the original domain, gives us a shallow water model that considers the possibility of a non constant bottom and the horizontal velocity components depend on z if the vorticity is not zero. This represents an interesting novelty respect to the shallow water models found in the literature. We stand out that we do not need to make *a priori* assumptions about velocity or pressure behavior to obtain the model.

The new model is able to calculate exactly the solutions of Euler equations that are linear in z, whereas the classic model just obtains the averaged velocities.

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The analytical calculations of the parameters of the fluctuations of the ballistic missiles. **Vladimir Gordon** (Orel State Technical University, Russian Federation), Pavel Anokhin (Orel State Technical University, Russian Federation), Svetlana Ovsyannikova (Orel State Technical University, Russian Federation) IC/CT4074/041

The analytical calculations of natural frequencies and forms of the longitudinal and flexural vibrations of the heterogeneous rods, which simulate ballistic missiles, are proposed. These objects are characteristic by significant drops in the distribution of stiffness and density along the length. The indicated dynamical characteristics knowledge is necessary for the design of the system of control and evaluation of the strength of articles.

Traditionally /1/ calculation is produced by the very labor-consuming method of sequential approximations.

It is proposed to use the analytical method, operational and effective for the arbitrary laws of distribution of stiffness and densities, for the purpose of the reduction of time and cost of dynamic calculations at the stage of preliminary design (selection of layout, sizes and materials).

The mathematical model of the dynamics of ballistic missile are differential equations of the second and the fourth orders with the variable coefficients and the corresponding boundary and initial conditions, and also different assumptions and limitation. The essence of the proposed method is based on the ideas of the asymptotic phase integral method of Wentzel-Kramers-Brillouin and method of Liouville-Steklova /2/. According to the proposed method the calculation of the natural frequencies of oscillation is reduced to the calculation of several dozens simple integrals. The comparison of the executed calculations with the results, obtained by approved traditional method shows the high accuracy of the proposed method (divergence $< 2\%$). Advantages of the method: analyticity, small labor expense, clarity, universality. For these reasons it is recommended for putting into practice of design.

Reference

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Numerics, characteristics, asymptotics: a case study from large-scale ocean circulation. **Frank Hodnett** (University of Limerick, Ireland) IC/CT504/171

This paper uses a partial differential equation which occurs in a reduced model of large scale circulation in an ocean basin as an educational vehicle through which to demonstrate the usefulness of a set of mathematical techniques in analyzing the equation. A parameter occurring in the equation does in reality vary from very small through intermediate to very large values. Therefore separate solutions are required for (a) very small, (b) very large and (c) intermediate values of the parameter. This allows for the demonstration of how, when the parameter is very small, the method of characteristics and the singular perturbation method are useful. When the parameter is very large the regular perturbation method is useful. At intermediate values of the parameter numerical methods must be used and in this case it is a helpful check to have available the asymptotic results for both small and large values of the parameter.

ŞWork done in collaboration with Colin CourtneyŤ

IC/CTS4599/04: PDEs: solutions and asymptotics.

Organiser: Giles Auchmuty (National Science Foundation, USA)

On the Stokes problem in cylinders becoming unbounded. **Sorin Mardare** (Universität Zürich, Switzerland), Michel Chipot (Universität Zürich, Switzerland) IC/CT2482/041

We establish that the solution to the Stokes problem in a cylinder becoming infinite in the direction of its axis converges to the solution to the Stokes problem defined on the basis of the cylinder, if the applied forces are orthogonal to the axis of the cylinder and independent of the coordinate along this axis.

Exact equations of motion for smoothed Wigner transforms and homogenization of wave propagation. **Agissilaos Athanassoulis** (Wolfgang Pauli Institut, Wien, Austria), Konstantinos Politis (National Technical University of Athens, Greece) IC/CT2582/041

In the study of wave propagation over distances much longer than the typical wavelength phase-space methods are often used, i.e. spectral densities are used as a homogenized representation of the wavefield, and kinetic equations are constructed for their evolution.
The Wigner Transform (WT) is a nonlinear, nonparametric spectral density, first introduced by E. Wigner in 1932 in the context of quantum mechanics. In the last ten years it has been extensively used in the formulation of phase-space models for a variety of problems, such as geometrical optics limits, periodic problems, nonlinear and/or random waves. Physical areas of application include semiconductors, linear and nonlinear optics, water waves and more.
However, the WT features counterintuitive interference components, which make computation and interpretation problematic. To face this, variants such as Wigner measures or Wigner spectra are typically used in practice.
We use smoothed Wigner Transforms (SWT) to study wave propagation. We present the derivation of new, to the best of our knowledge, exact equations of motion for the SWT covering a broad class of wave propagation problems. As a special case we get exact equations of motion for spectrograms of wave fields. These are typically pseudodifferential (i.e. integrodifferential) in leading order.
Finally, we use the new equations to build a numerical technique for computing on caustics Ű as opposed to before and after, but not really on, caustics, that the existing Wigner measures methods work for. We present some case studies; the results from our method are in very good agreement with full solutions of the corresponding problems.

Helmholtz equation outside an open arc in a plane with a mixed boundary condition. **Valentina Kolybasova** (Lomonosov Moscow State University, Russian Federation), Pavel Krutitskii (Keldysh Institute of Applied Mathematics RAS, Russian Federation) IC/CT3405/042

A boundary value problem for the Helmholtz equation

$$\Delta u - k^2 u = 0, \quad k = \operatorname{Re} k > 0$$

outside an open arc in a plane is studied with mixed boundary conditions. In doing so, the Dirichlet condition is specified on one side of the open arc and the boundary condition of the third kind is specified on the other side of the open arc. We consider non-propagative Helmholtz equation, real-valued solutions of which satisfy maximum principle. By using the potential theory the boundary value problem is reduced to a system of singular integral equations with additional conditions. By regularization and subsequent transformations, this system is reduced to a vector Fredholm equation of the second kind and index zero. It is proved that the obtained vector Fredholm equation is uniquely solvable. Therefore the integral representation for a solution of the original boundary value problem is obtained. The computational methods for finding the numerical solution are discussed.

Global spatial regularity of solutions of an elasto-viscoplastic model. **Dorothee Knees** (Weierstraß-Institut Berlin, Germany) IC/CT1291/042

We present a global spatial regularity result for the displacements u, stresses σ and inner variables z of a quasi-static model from elasto-viscoplasticity. The model under consideration reads as follows for a domain Ω and a time interval $S = (0, T)$:

$$\operatorname{div}\sigma(t) + f(t) = 0\,, \quad \sigma(t) = A(\varepsilon(u(t)) - Bz(t))\,, \quad \partial_t z(t) = g(\sigma(t), \varepsilon(u(t)), z(t))$$

together with an initial condition for z and Dirichlet- and Neumann-conditions on $\partial\Omega$. Here, A denotes the elasticity tensor and B is a linear mapping which maps the internal variable z on the inelastic strain. The function g is a constitutive function which is assumed to be Lipschitz-continuous. For example, models of this type result from the Yosida-approximation of elasto-plastic models with linear hardening.

Under suitable assumptions on the data, this system has a weak solution $u \in L^p(S; H^1(\Omega))$ and $z \in W^{1,p}(S; L^2(\Omega))$ for some $p \in [1, \infty]$. Our main result is the following: if the domain and the data are smooth enough, then the weak solutions have the global spatial regularity $u \in L^p(S; H^2(\Omega))$ and $z \in W^{1,p}(S; H^1(\Omega))$. This theorem is proved with a difference quotient technique. We discuss furthermore, in which way results for nonsmooth domains can be achieved from the results for smooth domains.

Cauchy problem for a higher-order Boussinesq equation. **Albert Erkip** (Sabanci University, Turkey), Nilay Duruk (Sabanci University, Turkey), Husnu Erbay (Isik Üniversitesi, Turkey) IC/CT1699/042

In this study we establish global well-posedness of the following Cauchy problem for a higher-order Boussinesq equation:

$u_{tt}-u_{xx}-u_{xxtt}+\beta u_{xxxxtt} = (g(u))_{xx}$, $x \in \mathbb{R}$, $t > 0$, $u(x,0) = \phi(x)$, $u(x,0) = \psi(x)$

where β is a positive constant, $u(x,t)$ is a real-valued function of two real variables and $g(u)$ is a given function of u with $g(u) = 0$.

At the microscopic level the higher order Boussinesq equation was derived[1] for the longitudinal vibrations of a dense lattice, in which a unit length of the lattice contains a large number of lattice points. Thus, in the above higher-order Boussinesq equation which has been written in terms of the scaled variables, $u = u(x,t)$ is the longitudinal strain, t is time and x is a spatial coordinate along the length of the lattice. The same equation may also be derived at the macroscopic level using the continuum mechanics approach, in particular the nonlocal elasticity theory that includes the effect of long range interatomic forces.

We first establish[2] local well-posedness of the Cauchy problem in the Sobolev space H^s with any $s > 1/2$. The contraction mapping principle is used to prove the following theorem about the local existence and uniqueness of the Cauchy problem:

Theorem *Assume that* $s > \frac{1}{2}, \phi \in H^s, \psi \in H^s$ *and* $g \in C^{[s]+1}(R)$ *with* $g(u) = 0$, *then there is some* $T > 0$ *such that the above Cauchy problem has a unique local solution* $u \in C^2([0,T], H^s)$.

Next we prove the following result about global existence:

Theorem *Let conditions of the first theorem hold with* $s \geq 1$. *Assume further that* ψ *is the derivative of some* L^2 *function and* $G(u) = \int_0^u g(s)\,ds \geq 0$ *for all* $u \in \mathbb{R}$. *Then the above Cauchy problem has a unique global solution* $u \in C^2([0,\infty), H^s)$.

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Variational principles for evolution equations. **Giles Auchmuty** (National Science Foundation, USA) IC/CT1973/042

This talk will describe variational principles that characterize the solutions of linear and nonlinear initial boundary value problems. These variational principles provide different methods for proving existence uniqueness theorems. Their construction depends on methods from convex analysis.

IC/CTS4931/04: Free-boundary problems.

Organiser: Juan Francisco Padial (Universidad Politécnica de Madrid, Spain)
Co-organiser: Lourdes Tello (Universidad Politécnica de Madrid, Spain)

Stability of the moving boundary in a non-equilibrium shrinking unreacted core model with fast reaction for the sphere. **Adrian Muntean** (Universität Bremen, Germany) IC/CT2801/045

Many reaction-diffusion scenarios taking place in unsaturated reactive porous materials involve the formation and propagation of moving-sharp interfaces, where fast chemical reactions are assumed to be concentrated. When spatially separated reactants meet, the separation boundary may be assumed as sharp provided that the characteristic time scale of reaction is much smaller than that of transport. We illustrate the shrinking core setting by means of a moving-boundary system with kinetic condition modeling the driving force. We employ this formulation in order to study the evolution of the reaction front in a sphere made of partially wet porous material. The model relies on the idea that the reaction might be considered to be localized on a sharp interface. It consists of a set of semi-linear mass-balance equations coupled with a non-linear ordinary differential equation, which accounts for the motion of the interface. We refer to this differential equation driving the sharp-reaction interface into the material as the *kinetic (non-equilibrium) condition*. The model equations are non-linearly coupled by the *a priori* unknown position of the moving-reaction interface and non-linearities in the production terms. We present results on the well-posedness of the model and discuss the practical relevance of some of the estimates. Special attention is granted to the stability of the interface position with respect to alterations in the model parameters.

Existence of solutions for an eigenvalue problem with weight. **Siham El Habib** (University Mohamed I, faculty of sciences, Oujda, Morocco), Najib Tsouli (Université Mohammed Premier Oujda, Morocco) IC/CT869/015

In this work we study the existence of solutions for the eigenvalue problem $\Delta_p^2 u = \lambda m(x)|u|^{p-2}u$, $u \in W^{2,p}(\Omega)$ in a bounded smooth domain Ω, with Neumann boundary condition $\frac{\partial u}{\partial \nu} = 0$ on $\partial\Omega$, and where $m \in L^r(\Omega)$, $m \neq 0$ is a weight function which can change its sign, with $r = r(N,p)$ satisfying the conditions: $r > \frac{N}{2p}$ for $\frac{N}{p} \geq 2$ and $r = 1$ for $\frac{N}{p} < 2$.

On the mathematical models of the shock between a viscoelastic bar and a body. **Arpad Takacsi** (Univerzitet u Novum Sadu, Yugoslavia) IC/CT722/015

In the paper by Bergounioux, M., Long, N.T., Dinh, A.P.N., *Mathematical model for a shock problem involving a linear viscoelastic bar*, Nonlinear Analysis, Theory, Methods & Applications, Vol. 43, 547–561, 2001, the authors introduced and analyzed mathematical models of the shock between a body and a viscoelastic bar. In this presentation, applying the Mikusiński operator calculus we obtain an ordinary differential equation in the operator field, $\mathcal{F}$, and then solving it obtain the exact and the approximate solution in $\mathcal{F}$. The classical exact and approximate solutions are obtained by inverting the previously obtained operator ones.

Crystal dissolution and precipitation in porous media: variable pore geometry and upscaled model. **Tycho Van Noorden** (Technische Universiteit Eindhoven, The Netherlands), Iuliu Sorin Pop (TU Eindhoven, The Netherlands) IC/CT2524/045

In this work we propose a pore scale model for crystal dissolution and precipitation in a porous medium. Using this model we derive a macroscopic model using a formal homogenization procedure. Our investigations are motivated by the work of P. Knabner et al. (*Adv. Water Res.* 1995) and C.J. van Duijn et al. (*J. reine angew. Math.* 2004).

We consider a porous medium that is fully saturated by a fluid in which cations (e.g. sodium ions) and anions (e.g. chlorine ions) are dissolved. In a precipitation reaction, n cations and m anions can precipitate in the form of one particle of crystalline solid (e.g. sodium chloride) attached to the surface of the grains (the porous matrix). The reverse reaction of dissolution is also possible. As a result of the precipitation and dissolution of crystals the geometry of the flow domain may change.

The model we propose consists of a system of coupled partial

differential equations on a variable domain. The changes in the flow domain, which occur due to the dissolution and precipitation of crystals are modeled by a one phase Stefan-like free boundary condition. This describes the movement of the interface between the fluid and the crystal layer.

For simple geometries we show that solutions of the pore scale model exist and we study their qualitative behavior using both analytic and numerical techniques. In addition we present a numerical study of the macroscopic model.

On some nonlinear elliptic problems with an unknown measure data. **Juan Francisco Padial** (Universidad Politécnica de Madrid, Spain) IC/CT4423/045

We introduce a new type of nonlinear elliptic problems

$$\mathcal{A}(u) = \mu(\cdot, u) \quad \text{and} \quad <\mu(\cdot,u), \varphi> = \int_{\partial u^{-1}(\{1\})} \varphi(y) q(y) dH_{N-1}(y)$$

for all $\varphi \in C(\bar{\Omega}) \cap V$ and where V is a reflexive Banach space, $\mathcal{A}$ is a pseudo monotone, coercive bounded operator from V into V^*, q is a positive continuous function on $\bar{\Omega}$ (Ω is a bounded open subset of $\mathbb{R}^N$, $N \geq 2$) and H_{N-1} is the $N-1$ dimensional Hausdorff measure. In constrast with the usual elliptic problems, the Radon measure μ is an unknown of the problem depending on the solution u. A particular cases of this type problems can be understood as a particular case of the *Bernoulli problem*: to look for a function $u : \Omega \subset \mathbb{R}^N \to \mathbb{R}$ and a subset $B \subset \mathbb{R}^N$ such that $-\Delta u = 0$ in $\Omega \setminus B$, $u = 0$ on $\partial\Omega$, $u = 1$ on $\partial\Omega$ and $\frac{\partial u}{\partial n} = q$ on ∂B. We will study the existence (by ussing the Ambrosetti–Rabinowitz maontain pass lemma) and non existence and the uniqueness of solutions for the cases described before (Díaz, Padial and Rakotoson, On some Bernouilli free boundary type problems for general elliptic operators. *To appear* in The Royal Society of Edinburgh Proceedings A (Mathematics)).

Blow-up results for fractional differential equations. **Mokhtar Kirane** (Université de La Rochelle, France) IC/CT4465/004

Blow-up results are presented for systems of fractional differential equations with cross-diffusion terms in space and time.

IC/CTS4606/04: Conservation laws, symmetries.

Organiser: Marco Mazzotti (ETH Zürich, Switzerland)

A new family of schemes for kinematic flows with discontinuous flux. **Raimund Bürger** (Universidad de Concepción, Chile) IC/CT971/046

In engineering applications, multiphase flows of suspensions and emulsions are frequently approximated by spatially one-dimensional kinematic models, in which the velocity of each species of the disperse phase is a given function of the vector of concentrations of all species. The continuity equations then form a system of conservation laws, which describes the spatial segregation of species. This class of models also includes multi-class traffic flow, where vehicles belong to different classes according to their preferential velocities. Recently, these models were extended to fluxes that depend discontinuously on the spatial coordinate. This situation appears, for example, in clarifier-thickener models and in traffic flow with variable road surface conditions.

This paper presents a new family of numerical schemes for such kinematic flows with a discontinuous flux. It is shown how a very simple scheme for the scalar case, which is adapted to the "concentration times velocity" structure of the flux, can be extended to kinematic models with a velocity that changes sign, flows with two or more species (the system case), and discontinuous fluxes. In addition, a standard MUSCL-type upgrade can be devised to attain second order accuracy. It is proved that system variants of the scheme preserve an invariant region of admissible concentration vectors, provided that all velocities have the same sign. Moreover, for a multiplicative flux discontinuity, it is proved that scalar versions converge to a BV_t entropy solution of the model. In the latter case, the compactness proof involves a novel uniform but local estimate of the spatial total variation of the approximate solutions.

Numerical examples all variants within the new family of schemes applied to abstract examplesand problems of sedimentation, traffic flow, and the settling of oil-in-water emulsions.

This presentation is based on joint work with A. García, K.H. Karlsen and J.D. Towers.

Entropy behaviour of evolution PDEs. **Phil Broadbridge** (AMSI, Australia) IC/CT4255/046

The concepts of entropy and of irreversibility can be introduced in a self-consistent manner and at an elementary level by reference to some simple evolution equations such as the linear heat equation. Given an evolving probability distribution p(x,t), the Shannon entropy is the expected value of log (1/p). This must increase monotonically if p(x,t) represents a thermodynamic process. In turn, this is equivalent to the density $p\ log(1/p)$ having a non-negative source term. This is easily seen to be true when p(x,t) satisfies a general nonlinear 2nd order diffusion equation.

When we consider fourth order diffusion terms, new problems arise. The fourth order equation $p_t = -p_{xxxx}$ is irreversible because the evolution operator is self adjoint with negative spectrum and therefore the locally defined density p^2 has a source term that is negative. However, the source term of -$p\ log|p|$ can take either sign. We know from applications such as thin film flow, and surface diffusion on metals, that fourth order diffusion terms always generate ripples rather than a monotonic approach to equilibrium. Despite this, we can construct a non-trivial class of fourth order quasilinear diffusion equations that increase the Shannon entropy and maintain positivity.

Similarity reductions of a nonlinear model for vibrations of beams. **Maria Santos Bruzon** (Universidad de Cádiz, Spain) IC/CT3435/046

The application of Lie transformations group theory for the construction of solutions of nonlinear partial differential equations is one of the most active fields of research in the theory of nonlinear partial differential equations and applications.

Motivated by the fact that symmetry reductions for many PDEs are know that are not obtained by using the classical symmetries, there have been several generalizations of the classical Lie group method for symmetry reductions. The notion of nonclassical symmetries was firstly introduced by Bluman and Cole to study the symmetry reductions of the heat equation. Clarkson and Mansfield proposed an algorithm for calculating the determining equations associated with the nonclassical method.

Symmetries and reductions technique are applied to a mathematical model which describe the vibrations of a beam.

Occurrence of a δ-shock in nonlinear chromatography. **Marco Mazzotti** (ETH Zürich, Switzerland) IC/CT1360/046

The local equilibrium model of two-component nonlinear chromatography consists of the following two first order partial differential mass balance equations (conservation laws): $u_t + f_t(u,v) + u_x = 0$ and $v_t + g_t(u,v) + v_x = 0$, where u and v are the concentrations of the species to be separated, and t and x are time and space. The solution for a Riemann problem (constant initial state in the column, and constant feed composition) consists of constant composition states separated by transitions, i.e. concentration fronts. The latter can be continuous simple waves that fulfill the partial differential equations or discontinuous shocks that fulfill the so called Rankine-Hugoniot condition, where no mass accumulation on the shock front is assumed.

We study the solution of Riemann problems, where adsorption of the two species is characterized by the following functions f and g defining the so called adsorption isotherms: $f(u,v) = au/(1-u+v)$ and $g(u,v) = bv/(1-u+v)$, where b and a, with $b > a$, are constant. In this case the model equations are of a mixed type, i.e. they are hyperbolic in a region of the composition space and elliptic in the remaining part of it.

It is shown that for some Riemann problems in the hyperbolic region the solution is not constituted of constant states separated by simple waves and shocks only. In these cases the Rankine-Hugoniot condition, that implies the conservation of mass through the shock with no accumulation on the shock itself, cannot be fulfilled. The solution can accommodate the excess mass only by admitting material accumulation on the shock, thus generating a spike that grows while traveling on top of the shock discontinuity along the column. Mathematically, this is a Dirac-delta, which in this context is called delta-shock.

On adaptive HRSC techniques for multi-class traffic flow problems. **Rosa Donat** (Universitat de València, Spain), Pep Mulet (Universitat de València, Spain) IC/CT2228/004

Multi-class traffic flow problems can be modeled as hyperbolic systems of conservations laws. The characteristic structure of these systems is seldom known, thus posing significant difficulties to schemes based on approximate Riemann solvers.

There has been recent interest in the application of "solverless" high resolution shock capturing (HRSC) schemes, such as those based on non-characteristic WENO (cf. [Zhang,Wong,Shu] and references therein), for which only an estimate of the maximum wave speed is needed. Results comparable to those obtained with monotone first-order schemes, such as Lax-Friedrichs, can be obtained with much coarser grids, and adaptive techniques can be used to lower the computational cost of the simulation (cf. [Burger,Kodacevicius]).

We present HRSC schemes that incorporate more characteristic information, together with an Adaptive-Mesh Refinement technique specifically designed for finite-differences WENO-like techniques. The fine resolution simulations one can achieve with the combination of these two techniques, show that there can be substantial differences between a non-characteristic scheme versus a characteristic-based scheme.

IC/CTS4608/04: Conservation laws, symmetries.

Organiser: Vladimir Shelkovich (Saint Petersburg State University, Russian Federation)
Co-organiser: Olga Rozanova (Moscow State University, Russian Federation)

Numerical solutions of population-balance models in particulate systems. **Shamsul Qamar** (Universität Magdeburg, Germany) IC/CT843/046

This work focuses on the derivation of numerical schemes for solving population balance models (PBMs) with simultaneous nucleation, growth and aggregation processes. The population balance equation is considered to be a statement of continuity. It tracks the change in particle size distribution as particles are born, die, grow or leave a given control volume. In the population balance models the one independent variable represents the time, the other(s) are *property coordinate(s)*; e.g., the particle size in the present case. They typically describe the temporal evolution of the number density functions and have been used to model various processes. These include crystallization, polymerization, emulsion and cell dynamics.

Two numerical methods are proposed for this purpose. The first method combines a method of characteristics (MOC) for growth process with a finite volume scheme (FVS) for aggregation processes. For handling nucleation terms, a cell of nuclei size is added at a given time level. The second method purely uses a semidiscrete finite volume scheme for nucleation, growth and aggregation of particles. Note that both schemes use the same finite volume scheme for aggregation processes. On one hand, the method of characteristics offers a technique which is in general a powerful tool for solving linear growth processes, has the capability to overcome numerical diffusion and dispersion, is computationally efficient, as well as give highly resolved solutions. On the other hand, the finite volume schemes which were derived for a general system in divergence form, are applicable to any grid to control resolution, and are also computationally not expensive.

In the first method a combination of finite volume scheme and the method of characteristics gives a highly accurate and efficient scheme for simultaneous nucleation, growth and aggregation processes. The second method demonstrates the applicability, generality, robustness and efficiency of high resolution schemes. The numerical test cases show clear advantages of the current schemes for the solution of population balances.

Symmetry analysis for a thin film type equation. **Maria Luz Gandarias** (Universidad de Cádiz, Spain) IC/CT1046/046

We consider the one-dimensional version of

$$u_t = -\nabla.(f(u)\nabla.(\Delta u)) - k\nabla.(g(u).(\nabla u)) = 0\,,$$

where u stands for the thickness of the film and f and g depends on the geometry of the problem. Such equations have been used to model the dynamics of a thin film of viscous liquid. The one dimensional equation

$$u_t = -(f(u)u_{xxx})_x - k(g(u)u_x)_x$$

applies if the liquid film is uniform in one direction. We analyze this equation by means of the theory of symmetry reductions of partial differential equations. It is found that some similarity solutions are solutions with physical interest.

Criterium for the gradient catastrophe for the non-isentropic gas dynamics equations. **Olga Rozanova** (Moscow State University, Russian Federation) IC/CT485/046

It is well known that the solutions of the systems of gas dynamics equations, being smooth initially, can lose the initial smoothness within a finite time (this phenomenon is called the gradient catastrophe. However, the sufficient and necessary conditions for the gradient catastrophe in the terms of initial data were known only for the isentropic one-dimensional flow, where one can write the system of two quasi-linear equations in the Riemannian invariants and then apply the method of char-

acteristics. In the non-isentropic case this criterium of such kind were known even for one space dimension. Nevertheless, some particular results are obtained, as usual, they concerns only sufficient conditions of the loss of smoothness (Sideris, Pokhozhaev).

We propose the method to describe the motion by means of integral functionals, which are actually integrals of the solution components over a material volume. Included among the functionals are the kinetic and potential energies, impulse, momentum of mass, and a number of specific integrals. These integral functionals are functions of time and satisfy a system of ODE, which is closed provided we consider a velocity field, linear inside of an infinitesimal material volume. Further, the problem about the data resulting the gradient catastrophe can be reduced to the problem of blow-up in a system of ODE for n^2 functions (which are derivatives of velocity), where n is the dimension of space. For $n = 1$ this system of ODE consists of one equation and can be investigated completely, therefore the criterium of the gradient catastrophe can be obtained. Moreover, the method gives a possibility to determine the place of arising singularity.

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The theory of δ- and δ'-shock wave type solutions to systems of conservation laws and the transportation and concentration processes. **Vladimir Shelkovich** (Saint Petersburg State University, Russian Federation) IC/CT427/046

There are *nonclassical* situations when systems of conservation laws admit δ- and δ'-shock type solutions. δ-Shock (δ'-shock) is a singular solution such that its components may contain the Dirac delta functions (the Dirac delta function and their derivatives). For the theory of δ-shocks see [1], [3], [4] and the references therein. An absolutely new theory of δ'-shocks was established in [5], [6].

1. By using [1], [3], [4], we describe the dynamics of propagation and interaction of δ-shock fronts in multidimensional zero-pressure gas dynamics in conservative form

$$\rho_t + \nabla \cdot (\rho U) = 0, \quad (\rho U)_t + \nabla \cdot (\rho U \otimes U) = 0,$$

non-conservative form

$$\rho_t + \nabla \cdot (\rho U) = 0, \quad U_t + (U \cdot \nabla) U = 0,$$

relativistic form

$$\rho_t + \nabla \cdot (\rho C(U)) = 0, \quad (\rho U)_t + \nabla \cdot (\rho U \otimes C(U)) = 0,$$

where $C(U) = \frac{c_0 U}{\sqrt{c_0^2 + |U|^2}}$, c_0 is the speed of light.

2. In the framework of the problems **1.** we derive δ-shock balance relations connected with mass and momentum transportation (from a volume into a singular surface).

We construct δ-shock wave type solution of the Cauchy problem for zero-pressure gas dynamics, describing the dimensional bifurcations of the singular support of this solution from $(n-1)$-dimensional surface into a point. These results can be used for description of transportation and concentration processes and may lead to discovery of new physical effects in cosmology.

3. For the system

$$u_t + (f(u))_x = 0, \quad v_t + (f_1(u)v)_x = 0, \quad w_t + (f_{22}(u)v^2 + f_{21}(u)w)_x = 0,$$

the Cauchy problems admitting δ'-shock is solved, where $f(u)$, $f_1(u)$, $f_{21}(u)$, $f_{22}(u)$ are smooth functions.

In order to deal with singular problems **1.**-**3.** the *weak asymptotics method* [2]–[4] is used.

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On a numerical solution of the Cauchy problem for the Laplace equation by the fundamental solutions method. **Takashi Ohe** (Okayama University of Science, Japan), Kohzaburo Ohnaka (Osaka university, Japan), Katsu Yamatani (Meijo University, Japan) IC/CT2929/047

Let Ω be an annular domain $\{\mathbf{x} \mid 0 < \rho_1 < |\mathbf{x}| < \rho_2\} \subset \mathbb{R}^2$, and $\Gamma_\Theta \equiv \{\mathbf{x} = (\rho_2 \cos\theta, \rho_2 \sin\theta), 0 \le \theta \le \Theta\}$ be a connected part of the outer boundary of Ω, where $0 < \Theta \le 2\pi$. Suppose f and g be analytic functions defined on Γ_Θ. We consider a numerical approximation method for the solution of a Cauchy problem for the Laplace equation $\Delta u = 0$ in Ω with Cauchy conditions $u = f$ and $\partial u/\partial r = g$ on Γ_Θ.

The Cauchy problem for the Laplace equation is known as an ill-posed problem and difficult to obtain a proper numerical solution. Many researchers studied a numerical method for the problem by various approaches, for example, based on the finite difference method, and the finite element method. Hon and Wei (2003) studied a method based on the fundamental solutions method for the case that the domain Ω is a disk, however, they did not consider the case of an annular domain.

In this talk, we investigate a numerical method based on the fundamental solutions method for an annular domain. For the case that Γ_Θ is the whole of the outer boundary, i.e. $\Theta = 2\pi$, we have proposed a method using 'inner' and 'outer' fictitious charges, and have shown some theoretical analysis on the uniqueness and convergence of the numerical solutions [Ohe and Ohnaka(2004)]. We develop our method for the case where Γ_Θ is a part of the outer boundary, i.e. $\Theta < 2\pi$, and investigate convergence and stability properties using numerical experiments.

On a boundary-value problem for the differential equation of second order with discontinuous coefficients. **Rizvan Pashayev** (Baku State University, Azerbaijan) IC/CT4170/050

Consider the boundary-value problem

$$-y'' + q(x)y = \lambda^2 \rho(x) y, \quad 0 < x < +\infty, \quad \text{with } y(0) = 0, \tag{1}$$

where the function $q(x)$ is real-valued and satisfies the condition $\int_0^\infty x\,|q(x)|\,dx < +\infty$, and $\rho(x)$ is a piecewise constant function

$$\rho(x) = \begin{cases} 1 & \text{for } a_2 \le x < +\infty, \\ \alpha_2^2 & \text{for } a_1 \le x < a_2, \\ \alpha_1^2 & \text{for } 0 \le x < a_1. \end{cases}$$

In the case of $\alpha_1 = \alpha_2 = 1$ (i.e., when $\rho(E) \equiv 1$), the inverse problem of scattering theory for this boundary-value problem was completely solved by V.A. Marchenko (1955). When $0 <$

$\alpha_1 = \alpha_2 \neq 1$ this problem was first studied by M.G. Gasymov (1977), but complete solution of the inverse scattering problem was obtained by I.M. Guseinov and R.T. Pashayev (2002). It turns out that having a discontinuity in the function $\rho(x)$ considerably influences the structure of representation of the lost solutions, and the main equation of the inverse problem.

In this talk we study the inverse problem of scattering theory for this boundary-value problem, in the range where $\alpha_i > 0$ but $\alpha_i \neq 1$ for each of $i = 1, 2$, and where $\alpha_1 \neq \alpha_2$.

IC/CTS4612/04: Inverse problems, ill-posed problems.

Organiser: Tom Lahmer (Universität Erlangen–Nürnberg, Germany)
Co-organiser: Hui Cao (RICAM Linz, Austria)

Modified Landweber iterations in a multilevel setting applied to the determination of nonlinear material parameters in piezoelectricity. **Tom Lahmer** (Universität Erlangen–Nürnberg, Germany), Barbara Kaltenbacher (Universität Stuttgart, Germany) IC/CT1538/047

An efficient solution of the inverse problem of identifying nonlinear dependencies in hyperbolic systems of PDEs, here piezoelectric material parameter curves, is the aim of this work. The dominant material tensor entries in the coupled field equations which describe the electromechanical interplay are approximated by functions depending on the physical field quantities electric field or mechanical stress. In order to solve this nonlinear and ill-posed problem of parameter curve identification efficiently, modified Landweber iterations (steepest descent and minimal error) will be studied. A multilevel approach is expedient due to the discretization of the unknown parameter curves and high computational efforts solving the forward problem (transient, nonlinear FEM computations). Theoretical investigations concerning convergence and regularization properties of the methods in a multilevel scenario will be presented, along with numerical results from an example in piezoelectricity.

A sampling method for electromagnetic scattering in a half-space. **Christoph Schneider** (Universität Mainz, Germany), Martin Hanke (Universität Mainz, Germany), Bastian Gebauer (RICAM Linz, Austria) IC/CT2705/047

We consider a simple (though fully three-dimensional) mathematical model for the electromagnetic exploration of buried, perfectly electrically conducting objects within soil underground. We assume to have two homogeneous half spaces $\mathbb{R}^3_+$, $\mathbb{R}^3_-$ connected by a flat interface Σ_0. We apply AC voltage of a fixed low frequency of some kHz to coils positioned on a sheet S parallel to the interface at constant height. Thereby we generate a time-harmonic electromagnetic field and measure the voltage which is induced within these coils due to the electromagnetic field. However, we take the voltage induced by the scattered field not the total field. The scattered field is the field scattered by the perfect conducting objects Ω, while the total field is the scattered field added to the field generated by the coils. We assume that the objects are completely buried in the soil (i.e. $\overline{\Omega} \subset \mathbb{R}^3_-$). Further on the complement of Ω within the soil is supposed to be simply connected. The factorization method applied to the underlying mathematics leads to a product of three operators $M = LFL^T$. M maps the voltages applied to the coils on the sheet S to measurements of the induced voltages due to the scattered field in these coils. The operators L and L^T are transposed operators. They map the voltages applied to the coils on the sheet to the electromagnetic field on the boundary of the scatterer and vice versa. Furthermore F represents a certain diffraction of the field at the boundary of the scatterer. This factorization justifies a sampling method for whether a point of interest is located inside a buried scatterer. Unfortunately, our data do not suffice completely to characterize Ω using the given range of M. However, we can characterize a subset Ω_1 of Ω and obtain an approximate image of the buried object(s).

Numerical procedures for the determination of the leading coefficient $a(x)$. **Hossein Azari** (Shahid Beheshti University, Iran) IC/CT4064/047

The aim of this talk is to study the parabolic inverse problem of determination of the leading coefficient in the heat equation with an extra condition at the terminal. After introducing a new variable, we reformulate the problem as a nonclassical parabolic equation along with the initial and boundary conditions. The uniqueness and continuous dependence of the solution upon the data are demonstrated, and then finite difference methods, backward Euler and Crank–Nicolson schemes are studied. It is proved that both numerical schemes are stable and convergent to the real solution. The results of some numerical examples are presented, which demonstrate the efficiency and rapid convergence of the methods.

Balancing principle for solving naturally linearized elliptic Cauchy problem. **Hui Cao** (RICAM Linz, Austria) IC/CT512/047

A classical ill-posed problem elliptic Cauchy problem is considered. By natural linearization we transform elliptic Cauchy problem into linear ill-posed operator equation. Discretization is applied as a regularization method (also known as self-regularization) to obtain a stable approximate solution. Balancing principle as an adaptive strategy is studied to choose appropriate discretization level. Numerical tests illustrate the theoretical results.

Adaptive choice of regularization parameter for nonlinear statistical inverse problems . **Mihaela Pricop** (Universität Göttingen, Romania), Thorsten Hohage (Universität Göttingen, Germany) IC/CT813/047

In this talk we consider statistical inverse problems described by nonlinear operator equations $F(a) = u$ where a is an element of a Hilbert space and u is an L^2-function. We construct an estimator $\hat{a}_n$ of a from measurements of u perturbed by random noise using nonlinear Tikhonov regularization in a Hilbert scale setting. For a-priori parameter choice strategy order-optimal rates of convergence for the mean-integrated square error $\mathbf{E}\|\hat{a}_n - a\|^2$ have already been obtained, but an a-posteriori parameter choice was not available in our setting. As the discrepancy principle is not applicable since we are dealing with stochastic noise, we develop an adaptive regularization parameter rule starting from the Lepskii principle which proves to have order-optimal MISE. Applications to parameter identification problems for elliptic differential equations are also given.

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The multi-dimensional refinement indicators algorithm for optimal parametrization. **Hend Ben Ameur** (University of Tunis, Tunisia) IC/CT1300/047

The estimation of distributed parameters in partial differential equations (PDE) from measures of the solution of the PDE may lead to under-determination problems. The choice of a parameterization is a usual way of adding a-priori information by reducing the number of unknowns according to the physics of the problem. The refinement indicators algorithm provides a fruitful adaptive parameterization technique that parsimoniously opens the degrees of freedom in an iterative way. We present a *new general form of the refinement indicators algorithm* that is applicable to the *estimation of multi-dimensional parameters* in any PDE. In the linear case, we state the relationship between the refinement indicator and the decrease of the usual least-squares data misfit objective function. We give numerical results in the simple case of the identity model, and this application reveals the *refinement indicators algorithm as an image segmentation technique*.

IC/CTS4616/04: Spectral problems, stability, scattering.

Organiser: Ian Wood (University of Aberystwyth, UK)

Stationary transport equations: the case of continuous spectrum. **Illya Karabash** (Donetsk, Ukraine) IC/CT902/048

We consider the abstract kinetic equation $d\psi/dx = -JL\psi$, $x \in [0,\infty]$, in a Hilbert space H. It is supposed that $J = J^* = J^{-1}$, $L = L^* \geq 0$, $\ker L = 0$. The following theorem is proved: if JL is similar to a self-adjoint operator, then an associated boundary problem has a unique solution. We apply this theorem to the stationary equation of Brownian motion and the stationary Kolmogorov-Chapman equation.

Scattering for open quantum systems. **Mark Malamud** (Donetsk, Ukraine) IC/CT926/048

We will discuss applications of new results on scattering matrices and dilations of maximal dissipative operators to some open quantum systems. In particular, we consider an application to a quantum transmitting Schrödinger–Poisson system (cf.[1]).

A main ingredient of our talk is a new formula for scattering matrix $S(\lambda)$ of a scattering system $\{L, L_0\}$ where $L_0 = A_0 \oplus T_0$ describes a situation where both subsystems corresponding to the operators $A_0 = A_0^*$ and $T_0 = T_0^*$ do not interact while $L = L^*$ takes into account an interaction of the subsystems.

In the case of transmitting Schrödinger–Poisson system we find a formula for scattering matrix $\{S(\lambda)\}$ of a scattering system $\{L, L_0\}$ by means of the corresponding Weyl functions on half-lines and discuss its connection with characteristic functions of a family of maximal dissipative extensions corresponding to transparent boundary conditions. Moreover, we show that under some natural assumptions a transmitting Schrödinger–Poisson system is uniquely determined by the scattering matrix mentioned above.

Our considerations are partially based on uniqueness results for Dirac type and matrix Sturm–Liouville operators (see [2,3]) as well as on some recent results on absolutely continuous and singular spectrum of self-adjoint extensions of symmetric operators[4] and on coupling method for construction of generalized resolvents from[5].

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Chebyshev expansion for the eigenfunctions of the almost-Mathieu operator. **Jesus Abderraman** (Univ. Politécnica de Madrid, Spain) IC/CT3621/048

Quasiperiodic super-lattices are widely used in nanotechnology. Their spectrum is often associated with one-dimensional Schrödinger operators - with ergodic potential unity. The Almost Mathieu operator [1] is a typical example. A difference equation related to this operator is Harper's:

$$\Psi_{n+1} + 2\lambda\cos(2\pi n\theta + \nu)\Psi_n + \Psi_{n-1} = \varepsilon\Psi_n.$$

Here, the Ψ_n's are energy eigenfunctions and λ is a real parameter. For integer θ, the eigenfunctions $\Psi_n = U_n(\frac{\varepsilon}{2} - \lambda\cos(\nu))$ are easily obtained: the $U_n(x)$ are Chebyshev polynomials of second kind. The spectrum has one band in the compact range $[-2+2\lambda\cos(\nu), 2+2\lambda\cos(\nu)]$. When $\theta = \frac{p}{q}$ is rational the spectrum has exactly q bands. For irrational θ, the ergodic case, the spectrum is amazing and very complicated. There has been a lot of work on this spectrum [2]. The eigenfunctions have solutions in form of determinants of sections of the Jacobi matrix associated with Harper's equation. By certain gauge invariance properties of Schrödinger's operator, it is enough to study the case $-1 \leq \lambda \leq 1$. Due to ergodicity, the spectrum is independent of ν. In a first analysis, take $\nu = 0$. Harper's equation is then

$$\Psi_{n+1} + 2\lambda T_n(\cos(2\pi\theta))\Psi_n + \Psi_{n-1} = \varepsilon\Psi_n.$$

To solve this equation, eigenfunctions are not expanded in powers of ε, but in a series in $T_n(\cos(2\pi\theta))$. The dependency on ε and λ is transferred to the coefficients of the expansion. This allows us to analyze some properties of Ψ_n solutions for $n \to \infty$.

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On fractional Fourier transform of ultra-distributions. **Bharat Bhosale** (University of Mumbai, India) IC/CT54/015

The fractional Fourier analysis is used for investigations of fractal structures; which in turn are used to analyze different physical phenomena. For instance, it has got the applications in optical engineering, as has been discussed by Alieva and Barbe and many others.

In this paper, the fractional Fourier transform is extended to ultra-distributions of compact support. For this purpose, we considered the space $E\check{S}(M_p;K)$ of ultra-distributions of compact support on which fractional FT is transformable. Analogous results to that of Paley–Wiener theorems are obtained for ultra-differentiable functions and ultra-distributions in the context of the fractional FT. At the end indicated few applications showing its edge over the other transforms.

Boundary-value spaces and M-functions for non-selfadjoint operators. **Ian Wood** (University of Aberystwyth, UK) IC/CT2527/015

We develop an extension of abstract boundary value spaces from selfadjoint to non-selfadjoint operators. The starting point is an adjoint pair of operators A and $\widetilde{A}$ in a Hilbert space H which satisfy an abstract Green formula:

$$(\widetilde{A}^*u, v)_H - (u, A^*v)_H = (\Gamma_1 u, \widetilde{\Gamma}_2 v)_{\mathcal{H}} - (\Gamma_2 u, \widetilde{\Gamma}_1 v)_{\mathcal{K}}.$$

where $\mathcal{H}$ and $\mathcal{K}$ are abstract boundary spaces. Given $B \in \mathcal{L}(\mathcal{K}, \mathcal{H})$, the M-function (generalised Dirichlet to Neumann map) is defined by

$$M_B(\lambda) : \mathrm{Ran}\,(\Gamma_1 - B\Gamma_2) \to \mathcal{K},\ M_B(\lambda)(\Gamma_1 - B\Gamma_2)u = \Gamma_2 u \text{ for all } u \in \ker(\widetilde{A}^* - \lambda).$$

We then study the relationship between the M-function and spectral properties of realisations of $\widetilde{A}^*$. In particular, the results can be applied to elliptic operators.

Stability of vortices in 3D Bose–Einstein condensates. **Richard Kollár** (University of Michigan, Ann Arbor, Slovakia) IC/CT790/048

The structure of the nonlinear Schrödinger equation supports existence of topologically non-trivial vortex solutions. Their stability is studied by means of a very robust method – the Evans function. A traditional limitation of the Evans function technique is that it is generically an one-dimensional method and its extenstion to higher dimensions is very rare. In the case of the axi-symmetrical vortices in three-dimensional Bose-Einstein condensates we are able to extend this method by using information on Krein signature of eigenvalues.

04: Partial Differential Equations, Posters

IC/PP539/004: A combined Chebyshev polynomials and Sumudu transform for solving the neutron transport equation.

Presenter: Abdelouahab Kadem (Université Sétif, Algeria)

In this work, we present a new approximation for the one-group linear transport equation with anisotropic scattering in a slab, using Chebyshev polynomials. To this end, the angular flux is expanded in a truncated series of Chebyshev polynomials in the angular variable. Replacing this expression in the transport equation and taking moments like in the P_N method, leads to a new approximation. The resultant first-order linear differential system is solved for the spatial function coefficients by application of the Sumudu transform technique. The inversion of the transformed coefficients is performed also analytically, using Trzaska's method and the Heaviside technique.

IC/PP3980/040: Overlapping operator splitting methods and applications in stiff differential equations.

Presenter: Juergen Geiser (Humboldt-Universität zu Berlin, Germany)

We present the stability of an overlapping operator-splitting method based on overlapping iterative methods. We discuss the iterative Operator Splitting method in the context of decoupling the stiff and non-stiff operators with respect to overlap them. In the context of stabilization the stiff operators, we present the overlapping ideas as extension to the standard iterative operator splitting method. The efficiency of considering the overlapping method instead of the standard method is further discussed. We apply our theoretical results on model problems for stiff linear and nonlinear parabolic partial differential equations.

IC/PP4367/040: Behavior of solutions for a reaction–diffusion equation related to a model of crystal growth.

Presenter: Toshiko Ogiwara (Josai University, Japan)

We shall investigate a reaction–diffusion equation

$$u_t = u_{xx} + f(u), \quad x \in \mathbb{R}, \quad \text{for } t > 0,$$

where $f(u)$ is a periodic function with period 1. This is related to a mathematical model of crystal growth. Here the unknown function $u(x,t)$ represents the local height of the crystal surface and is normalized in order that 1 denotes the size of a unit molecule.

A solution $u(x,t)$ of this equation is called a *travelling wave* if it is written in the form $u(x,t) = \phi(x - ct)$ for some constant c and some function $\phi(y)$. Here we call the constant c the speed, and the function $\phi(y)$ the profile of the travelling wave.

We show that, for any $l > 0$, there exists a travelling wave $\phi(x - ct)$ with unbounded profile $\phi(y)$ satisfying

$$\phi(y - l) = \phi(y) + 1, \quad y \in \mathbb{R},$$

and consider the relation between the length l and the speed c. Furthermore, we study the asymptotic behavior of solutions with bounded initial data.

IC/PP4720/041: On the stability of damped Timoshenko systems: Cattaneo versus Fourier law.

Presenter: Hugo Danilo Fernandez Sare (Universität Konstanz, Germany)
Co-author: Reinhard Racke (Universität Konstanz, Germany)

We consider vibrating systems of hyperbolic Timoshenko type that are coupled to a heat equation modeling an expectedly dissipative effect through heat conduction. While exponential stability under the Fourier law of heat conduction holds, it turns out that the coupling via the Cattaneo law does not yield an exponentially stable system. This seems to be the first example that a removal of the paradox of infinite propagation speed inherent in Fourier's law by changing to the Cattaneo law causes a loss of the exponential stability property. Actually, for systems with history, the Fourier law keeps the exponential stability known for the pure Timoshenko system without heat conduction, but introducing the Cattaneo coupling even destroys this property.

IC/PP919/041: On the boundedness and compactness of a class of Fourier integral operators.

Presenter: Abderrahmane Senoussaoui (Université d'Oran Es-Sénia, Algeria)

We study the L^2-boundedness and L^2-compactness of a class of Fourier integral operators of types:

$$A\varphi(x) = \int_{\mathbb{R}^n} e^{iS(x,\theta)} a(x,\theta) \mathcal{F}\varphi(\theta)\, \mathrm{d}\theta\,,$$

in which appears two C^∞-functions, namely the phase function $S(x,\theta)$ and the amplitude a, and where $\mathcal{F}$ is the Fourier transformation.

These operators are bounded (respectively compact) if the weight of the amplitude is bounded (respectively tends to 0).

IC/PP1058/042: On some doubly nonlinear elliptic–parabolic equations in Banach spaces.

Presenter: Tomomi Kojo (Shibaura Institute of Technology, Japan)

We consider the IVP for some doubly nonlinear elliptic-parabolic equations of the form $d(Bu)/dt + Au = f$ in Banach spaces. Existence theorem of weak solutions for this equation is shown. Time discretization method is used to construct approximate solutions. Concerning the strong convergence of approximate solutions, we shall use a new type of compactness theorem.

IC/PP4048/043: Numerical solution for the diffusion equation subject to purely integral conditions.

Presenter: Souad Bensaid (University Centre Larbi Ben M'Hidi, Algeria)

In this paper, numerical schemes are developped for obtaining approximate solutions to the initial-boundary value problem for one-dimensional diffusion equation with purely integral conditions. These numerical schemes are based on the standard backward Euler method, the standard Crank-Nicholson method, a modified backward Euler method, and a modified Crank-Nicholson method. Some experimental numerical results using the proposed numerical procedure are discussed.

IC/PP4046/043: Galerkin method applied to parabolic problem with a nonlocal boundary condition.

Presenter: Abdelfatah Bouziani (University Centre Larbi Ben M'Hidi, Algeria)

The present paper is devoted to the investigation of a model parabolic mixed problem with boundary integral condition. Existence, uniqueness and continuous dependence upon data of a weak solution of this latter are proved by means of the Galerkin method.

IC/PP481/043: Boundary-value problem for higher-order parabolic evolution equations.

Presenter: Assia Guezane Lakoud (Annaba University, Algeria)
Co-author: Belakroum Dounia (University of Annaba, Algeria)

In this poster we will study a boundary value problem for higher order parabolic equations with unbounded operator coefficient in a Hilbert space. The proofs are based on *a priori* estimates. In appropriate functional spaces, we prove the existence, uniqueness and the continuous dependence of the strong solution to respect to data.

IC/PP4344/045: On a numerical scheme for the Willmore flow.

Presenter: Tomáš Oberhuber (Czech Technical University, Prague, Czech Republic)

The contribution deals with the Willmore flow which is described by the relaxation of a functional depending on the mean curvature of a curve or a surface. This problem comes from the physics of elasticity but there are also applications of the Willmore flow in image processing. We describe a numerical scheme based on the finite-difference method on a uniform grid. We deliver several qualitative examples of computation using the derived scheme as well as numerical studies of convergence demonstrating ability of the scheme.

IC/PP3127/046: Lie and conditional symmetries of systems of reaction–diffusion–convection equations.

Presenter: Roman Cherniha (National Academy of Sciences of Ukraine, Kyiv)

Systems of nonlinear reaction-diffusion-convection (RDC) equations of the form:

$$\bar{U}_t = (A(\bar{U})\bar{U}_x)_x + B(\bar{U})\bar{U}_x + \bar{C}(\bar{U})\,, \qquad (1)$$

where $\bar{U} = (U_1, U_2)$ is an unknown vector function, $\bar{C}(\bar{U}) = (C_1(\bar{U}), C_2(\bar{U}))$ is an arbitrary vector function, $A(\bar{U})$ and $B(\bar{U})$ are matrices 2×2 with the elements $a_{ij}(\bar{U})$ and $b_{ij}(\bar{U})$, $i,j = 1,2$ being arbitrary smooth functions, are considered. Systems of the form (1) describe a great number of various processes in physics, biology and chemistry. While there is no existing general theory for analytical integrating nonlinear RDC systems of the form (1), construction of particular exact solutions for these equations is a non-trivial and important problem. Finding exact solutions that have a physical, chemical or biological interpretation is of fundamental importance. Now the most powerful methods for construction of exact solutions to nonlinear RDC systems are the group-theoretical approaches.

Since a *complete description* of the Lie and conditional symmetries of system (1) is a very difficult problem in the general case, we present the recent results [1]-[5] obtained for several important subclasses of (1).

[1] Cherniha R.; Lie Symmetries of Nonlinear Two-dimensional Reaction–Diffusion Systems, Rept. Math. Phys., vol.46 (2000), pp.63–76.

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[3] Cherniha R. and King J.R.; Lie Symmetries and Conservation Laws of Nonlinear Multidimensional Reaction–Diffusion Systems with Variable Diffusivities. IMA J. Appl. Math., vol.71 (2006), pp.391–408.

[4] R. Cherniha and M. Serov; Nonlinear Systems of the Burgers-type Equations: Lie and Q- conditional Symmetries, Ansätze and Solutions. J.Math.Anal.Appl. 282 (2003), pp.305–328.

[5] R. Cherniha and O. Pliukhin; Conditional Symmetries of Nonlinear Reaction–Diffusion Systems with Power diffusivities. in preparation.

IC/PP1043/046: On bounded weak solutions of a degenerate parabolic equation.

Presenter: Young-Sam Kwon (American Mathematical Society, USA)

In this paper we consider bounded weak solutions u of a degenerate parabolic equation defined in a subset $(0,T)\times\Omega\subset\mathbb{R}^+\times\mathbb{R}^d$. We define a strong notion of trace at the boundary $(0,T)\times\partial\Omega$ reached by L^1 convergence for a large class of functionals of u. Those functionals depend on the flux function of the degenerate parabolic equation and on the boundary.

IC/PP4260/046: Strong trace for solutions of degenerate parabolic–hyperbolic equation.

Presenter: Young-Sam Kwon (American Mathematical Society, USA)

In this paper we show the existence of strong trace for entropy solutions of degenerate parabolic-hyperbolic equation on boundary of a bounded domain with smooth boundary.

IC/PP3075/047: On new analytical approach to some classes of mathematical physics inverse problems.

Presenter: Sharif Guseynov (Latvijas Universitate, Latvia)

The problems for partial differential equations are characterized by the main equation, the definition's domain, boundary and initial conditions. Therefore we can mark out coefficient, geometrical, boundary and evolutional inverse problems. In this paper we consider a some classes of non-homogeneous coefficient inverse heat transfer problems in the bounded domain under some additional information. In the coefficient inverse problems the coefficients of main equation and (or) or right-hand side are not known and have to be determined. Heat transfer inverse problems are manifold by appearances and forms of problems setting, by degree of incorrectness. Thus, these problems are suitable for approbation of the regularization theory methods and algorithms. The increase of interest in the solutions of these inverse problems is due to the needs of practices in connection with wide spread occurrence of non-stationary and nonlinear real heat-mass transfer processes. These effects require creation of the new mathematical approaches and methods (including analytical methods). The principal advantages of these methods are well known: they allow carrying out experimental researches, which are to the utmost zoomed-in to the real circumstances, or in time of the direct exploitation of technical objects. Determination of the thermal diffusivity is a rather challenging problem even for a homogeneous medium. We offer one simple analytical approach for determination of required coefficient of thermal conductivity under various type additional conditions. Offered approach lets reduce the initial inverse problem to the problem for the solution of the first kind Volterra linear integral equation. In the present work as example, we apply offered approach to steady-state inverse thermal conductivity problem. Let us note the offered method is suitable for solution of some classes of nonlinear direct and inverse problems of mathematical physics.

IC/PP3318/047: Inverse modelling: different methods.

Presenter: Evgeniy Tantserev (Universitetet i Oslo, Norway)

The transient heat conduction is generally described by the parabolic heat conduction equation for given initial temperature and boundary conditions, is well-posed problem with smooth dependence of results on initial data. However, many practical problems require solving heat conduction problem when based on final temperature distribution one has to find initial distribution. This problem is proven to be ill-posed and initial imperfections, even very small, will grow large during backwards evolution. There are some regularization techniques (for example, approximation of Lattes&Lions, Tiba, pseudo-parabolic) which approximate our ill-posed problem by well-posed problem. These techniques add regularization terms in original equation.

These terms are scaled by small regularization parameter, ϵ, and the solutions of regularized equations converge to the solution of original with $\epsilon\to 0$. However, if $\epsilon\neq 0$ two approaches, original backwards heat conduction problem (BHCP) and regularized BHCP may differ significantly. Thus, we need to understand when we can expect that regularized equations give acceptable approximation of BHCP. And we want to compare and understand acceptability of each of three methods: 1) quasi-reversibility (Lattes&Lions, 1969), 2) elliptic (Tiba, 1995), 3) pseudo-parabolic (Samarskii). If ϵ grows then the solutions of our regularized equations are stable but error of difference between two solutions (regularized and original) grows. If ϵ is very small regularization procedure is not effective, and some small initial perturbations grow exponentially with time. For each method we plot phase-diagrams which show the optimal choice of regularization terms. We compare these methods on one phase diagram in which domain what method is the best (for what method analytical solution of perturbed BHCP is nearest to analytical solution of BHCP for different frequencies and regularization parameters). For numerical solutions of these regularized problems we plot diagrams for few different frequencies which analyze their convergent, proximity to the analytical solutions that is show which method better for different parameters. After that we introduce another much known method, the iterative method, and in the end a mix of both types of methods to get a good solution of our backwards heat conduction problem.

IC/PP2091/048: An application of scaling inequality in nonlinear PDEs: an example of global stabilization of Burger's equation.

Presenter: Selvaraj Marshal Anthoni (Periyar University, India)

In this paper, we consider the problem of Neumann and Dirichlet control of Burger's equation. The purpose is to derive boundary control laws which make the system globally asymptotically stable. Scaling inequality is used for achieving the required robustness in Lyapunov-based stabilization. Especially this paper focuses on a new freedom of scaling with respect to spatial variables, which is naturally useful to nonlinear PDE's.

IC/PP777/015: A generalized Paneitz–Branson type equation on complete manifolds.

Presenter: Youssef Maliki (University Abou Bekr Belkaïd of Tlemcen, Algeria)

Let (M, g) be an n-dimensional Riemannian manifold with $n \geq 5$. The well known Paneitz–Branson type equation is of the form

$$\Delta_{\tilde{g}}^2 u - \operatorname{div}\Big(\frac{(n-2)^2}{2\,(n-1)\,(n-2)}\operatorname{scal}_g - \frac{4}{n-2}\operatorname{Ricc}_g\Big)\mathrm{d}u + \frac{n-4}{2}Q_g\,u = \frac{n-4}{2}Q_{\tilde{g}}\,u^{\frac{n+4}{n-4}}$$

where Δ_g is the Laplace–Beltrami operator, $Q_g = \frac{1}{2(n-1)}\Delta_g \operatorname{scal}_g + \frac{n^3-4n^2+16n-16}{8(n-1)^2(n-2)^2}\operatorname{scal}_g^2 - \frac{2}{n-2}\,|\operatorname{Ricc}|^2$ and $\tilde{g}$ is a conformal metric to g.

This equation is related with the study of the so-called Q-curvature; that is, a positive smooth solution provides a metric conformal to the background metric g, with the prescribed Q-curvature.

For $1 < p < \frac{1}{2}n$, we consider the following generalization:

$$\Delta_{\tilde{g}}^2\left(\left|\Delta_g\right|^{p-2}\Delta_g u\right) - \operatorname{div}\left(a(x)\,\left|\nabla_g u\right|^{p-2}\nabla_g u\right) + b(x)\,|u|^{p-2}\,u = f(x)\,|u|^{\frac{np}{n-2p}-2}\,u$$

Our aim is to solve this new equation on complete non-compact Riemannian manifolds. We prove that under some conditions on the geometry of the manifold together with conditions on the decay of the function f at infinity, this equation admits a weak solution.

05: Applied Analysis, Minisymposia

IC/MP4401/015: Mathematical aspects of materials science: plasticity and fracture.

Organiser: Antonio DeSimone (SISSA, Trieste, Italy)
Co-organiser: Stefan Müller (Max-Planck-Institut Leipzig, Germany)

See minisymposium IC/MP53/015 on page 393.

Rigidity results for cracked bodies. **Antonin Chambolle** (École Polytechnique, France) IC/MT1451/015

I will present exact rigidity results in the class of SBV functions and SBD displacement, which model respectively deformations and small displacements of cracked bodies, with discontinuities. For the first class, it is reasonable to wonder whether a deformation whose gradient is a.e. a rotation is "piecewise" affine (and piecewise a rigid deformation). For the second class, the natural question is whether $e(u) = 0$ (the absolutely continuous part of the symmetrized distributional gradient) implies also that u is piecewise rigid. In both cases, the answer is false without additional assumptions, thanks to a result of Alberti. We show that if the total surface of the jump set is finite, the answer to both questions is positive. The proof is based on a simplification technique, based on slicing, which turns functions with arbitrary jump set (but of finite measure) into nice functions with piecewise affine jump. In the SBD case, it is sufficient to deduce the rigidity. In the SBV case, it gives only some information on the curl of the approximate gradient. The conclusion then follows from a quantitative rigidity estimate in $W^{1,p}$ of Friesecke, James and Müller, together with an approximation argument borrowed from their proof. This is a work in collaboration with A. Giacomini and M. Ponsiglione.

Quasi-static evolution problems in plasticity with softening. **Gianni Dal Maso** (SISSA, Trieste, Italy) IC/MT3437/015

In plasticity theory the term softening refers to the reduction of the yield stress as plastic deformation proceeds. We deal with this problem in the quasistatic case, in the framework of small strain associative elastoplasticity. The presence of a nonconvex term due to the softening phenomenon requires the extension of a variational framework proposed by Mielke to the case of a nonconvex energy functional. In this problem the use of global minimizers in the corresponding incremental problems is not justified from the mechanical point of view. We analize a different selection criterion for the solutions of the quasistatic evolution problem, based on a viscous approximation. In view of the nonconvexity of the problem, taking the limit as the artificial viscosity parameter tends to zero leads to a weak formulation of the problem in a space of Young measures. Moreover, since the growth exponent of the energy is one, we need a suitable notion of generalized Young measure in order to deal with concentration effects. Finally, the classical notion of total variation of a time-dependent function on a time interval has to be extended to time-dependent families of Young measures. This enables us to define, in this generalized context, a notion of dissipation, which plays a crucial role in Mielke's variational approach. Some examples show that smooth initial data may lead, after a critical time, to a Young measure solution with concentration phenomena.

These results have been obtained in collaboration with Antonio DeSimone, Maria Giovanna Mora and Massimiliano Morini.

Existence of energetic solutions in finite-strain plasticity. **Alexander Mielke** (Weierstraß-Institut Berlin, Germany) IC/MT3585/015

Most theories of finite-strain elastoplasticity are based on Kröner and Lee's assumption of the multiplicative decomposition $\nabla\varphi = F_{\text{elast}}P^{-1}$ of the gradient of the deformation $\varphi : \Omega \to \mathbb{R}^d$. The plastic tensor P and additional hardening variables $p \in \Pi$ are taken to be internal parameters. Moreover, the modeling is usually done in the rate-independent setting. This talk concerns the implications of these two basic axioms. Our analysis uses the *energetic formulation* in its recent abstract form [1,4]. It is solely based on the *energy functional*

$$\mathcal{E}(t,\varphi,P,p) = \int_\Omega W_{\text{elast}}(x,\nabla\varphi P^{-1},p)+W_{\text{hard}}(x,P,p)dx+G_{\text{reg}}(P,p)-\langle \ell(t),\varphi\rangle$$

and the *dissipation distance* $\mathcal{D}((P_0,p_0),(P_1,p_1)) = \int_\Omega D(x,(P_0,p_0),(P_1,p_1))dx$. If $\mathcal{F}$ is the set of kinematically admissible deformation and $\mathcal{Z}$ is the set of all internal states, we call a function $(\varphi,P,p) : [0,T] \to \mathcal{F}\times\mathcal{Z}$ an *energetic solution*, if for all $t \in [0,T]$ the global stability (S) and the energy balance (E) hold:

(S) $\forall\,(\psi,Q,q) \in \mathcal{F}\times\mathcal{Z}$: $\mathcal{E}(t,\varphi(t),P(t),p(t))$
$hspace*{11em} \le \mathcal{E}(t,\psi,Q,q)+\mathcal{D}(P(t),p(t),Q,q)$,

(E) $\mathcal{E}(t,\varphi(t),P(t),p(t)) + \text{Diss}_{\mathcal{D}}((P,p),[0,T])$
$hspace*{7em} = \mathcal{E}(0,\varphi(0),P(0),p(0)) + \int_0^t \partial_s\mathcal{E}(s,\varphi(s),P(s),p(s))ds.$

We address the question under what conditions we can find such energetic solutions, or as a preliminary result we discuss existence of solutions to the associated incremental minimization problems. Our results strongly depend on the regularizing term G_{reg}. The case without regularization is treated in [3], a term involving $\text{curl}P$ is discussed in [5], and regularizations involving $(\nabla P,\nabla p)$ are treated in [2].

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[3] A. Mielke; Existence of minimizers in incremental elastoplasticity with finite strains. *SIAM J. Math. Anal.*, 36, pp.384–404, 2004.

[4] A. Mielke; Evolution in rate-independent systems (ch. 6). In "C. Dafermos, E. Feireisl (eds) *Handbook of Differential Equations, Evolutionary Equations, vol. 2*, Elsevier 2005", pp.461–559.

[5] A. Mielke, S. Müller; Lower semicontinuity and existence of minimizers for a functional in elastoplasticity. *ZAMM*, 86, pp.233–250, 2006.

This is partially joint work with Andreas Mainik and Stefan Müller.

Energy-dissipation functionals in fracture mechanics: crack branching and the mother–daughter mechanism. **Christopher Larsen** (Worcester Polytechnic Institute, USA), Michael Ortiz (California Institute of Technology, USA) IC/MT5054/015

Motivated by the idea that energy dissipation due to crack propagation occurs at crack fronts and might depend nonlinearly on propagation speed, we sought reasonable definitions for crack *front* and *front speed* and then analyzed energy-minimization models for crack trajectories. For a crack trajectory $t \mapsto C(t) \subset \Omega$, we say that at each time $t \in [0,T]$ the crack has front $F(t)$ with speed $v(x,t)$ if F and v satisfy the following:

$$\int_0^T \dot\varphi(t)\int_{C(t)} f(x)\mathrm{d}\mathcal{H}^{N-1}(x)\mathrm{d}t = -\int_0^T \varphi(t)\int_{F(t)} f(x)v(x,t)\mathrm{d}\mathcal{H}^{N-2}(x)\mathrm{d}t$$

$\forall\varphi \in C_{01}([0,T]), \forall f \in C_0(\Omega)$, with $F(t)$ being the minimal such set.

For this definition, discrete-time minimization is not very natural, and we turn instead to a model introduced by Mielke and

Ortiz for energy-minimizing trajectories. There are several issues in proving existence, mostly due to compactness problems for crack trajectories satisfying this equation. We will describe these issues (some of which involve mother–daughter cracks), as well as an existence result for a constrained problem and relaxation results for unconstrained problems.

This is joint work with M. Ortiz and C.L. Richardson.

IC/MP617/015: Microstructures, PDE and applications.

Organiser: Robert Lipton (Louisiana State University, USA)
Co-organiser: Alain Damlamian (Université Paris XII, France)

Microstructured materials appear naturally and are increasingly being adopted for use in the applications. The rapidly growing number of applications and contexts for microstructured materials, including those with optimal properties, provides new challenges for modeling and theory. The objective of this minisymposium is to provide a forum for the latest trends and methods used to quantify physical phenomena associated with microstructured media. The mathematical techniques covered in this symposium include homogenization theory, gamma convergence multi-scale numerical methods, regularity theory and methods for local field construction. The application areas include, imaging, composites, biological structures, optimal design, and phase transformations.

Homogenization of the Hall effect in dimension 2 and 3. **Marc Briane** (INSA Rennes, France) IC/MT1303/015

The present work is the fruit of a collaboration with G. Milton, and deals with the homogenization of the Hall effect in two and three dimensions. In Physics it is known that a low (constant) magnetic field induces a non-symmetric perturbation in the resistivity of a conductive material. When the material has a prescribed microstructure, Bergman derived in particular cases the effective (or homogenized) Hall effect from the one of the original microstructure combined with some currents in absence of magnetic field. In this work we extend the Bergman approach to any microstructure in the framework of the Murat-Tartar H-convergence. Moreover, we give some properties of the effective Hall effect. In dimension two we prove in collaboration with D. Manceau that the Hall effect reduces to one coefficient called the Hall coefficient, and that the homogenization process preserves the sign of the Hall coefficient. The three-dimensional case is more delicate. On the one hand, the Hall effect is now represented by a whole 3×3 matrix. On the other hand, the two-dimensional positivity property does not hold in dimension three. Indeed, we build a new microstructure with many symmetries associated with a positive isotropic Hall matrix such that the effective Hall matrix is still isotropic but negative.

Applications of homogenization techniques to the electrical conduction in biological tissues. **Micol Amar** (Università degli Studi di Roma “La Sapienza", Italy), Daniele Andreucci (Università degli Studi di Roma “La Sapienza", Italy), Paolo Bisegna (Università degli Studi di Roma Tor Vergata, Italy), Roberto Gianni (Università degli Studi di Roma “La Sapienza", Italy) IC/MT1711/015

It is well known that electric potentials can be used in diagnostic devices to investigate the properties of biological tissues. Such techniques are essentially based on the possibility of determining the physiological properties of a living body by means of the knowledge of its electrical resistance. This leads to an inverse problem for the Laplace equation, which is the standard equation, when only a resistive behavior of the body is assumed. However, it has been observed that, applying high frequency alternating potentials to the body, a capacitive behavior takes place. This effect (known in physics as Maxwell-Wagner effect) is due to the electric polarization at the interface of the cell membranes, which act as capacitors, and it has been studied, among others, by the authors, who assume that the biological tissue is modeled as a composite media with a periodic microscopic structure composed by two finely mixed phases (intra and extra cellular) separated by an imperfect interface (cellular membrane).

The mathematical description of the passage of the electrical current trough the tissue is given by a system of decoupled elliptic equations in the two phases, whose solutions are coupled because of the interface conditions, since they have to satisfy the property of flux-continuity and a transmission condition of dynamic type. The homogenization theory is used in order to pass from this microscopic description to the macroscopic one, which is given by a new equation, replacing the elliptic one used up to now.

Actually, other different microscopic models have been proposed in the literature, in order to take into account these capacitive effects. These models are obtained by different scalings (with respect to the characteristic dimension of the cell) of the parameters defining the physical behavior of the cell membranes and they lead to different macroscopic equations.

The authors discuss and compare these different models and investigate how microscopic mathematical descriptions can be obtained from the Maxwell equations in the quasi-stationary approximation. This analysis presents a unified derivation of different schemes, thus allowing a comparison among their underlying physical assumptions, and could be useful to assess the viability of each scheme as a model for a specific experimental setting.

Asymptotics for the voltage potential in a periodic network with localized defects. **Eric Bonnetier** (Université Grenoble I, France) IC/MT2188/015

We consider the restriction to an open bounded set Ω of the square lattice $h\mathbf{Z}^2$ as a network of conductors. In the reference configuration, each lattice point is connected to its 4 closest neighbors by a link of conductivity k. In a perturbed configuration, some of the links far from the boundary are defective and have conductivities $k_d \neq k$. Given a current flux on $\partial\Omega$, we compare the potentials u_h and $u_{h,d}$ of the reference and perturbed configurations. We show that at a point z far from the defective zone the potential difference has the form

$$u_{h,d}(z) - u_h(z) \quad = \quad h^2 \sum_i M_i : \nabla u(x_i) \otimes \nabla G(x_i, z) \; + \; o(h^2).$$

In this expression, x_i denotes the location of the i-th defect and h the lattice size. The matrix M_i is a polarization term, ∇u is the potential of the continuous effective medium obtained when $h \to 0$, and G is the Green's function associated to this same limiting effective medium. Thus, the expansion of $u_h - u_{h,d}$ has the same structure as the expansions derived when a smooth medium is perturbed by inclusions of small sizes, and for which efficient numerical detection algorithms have been proposed, taking advantage of the singular character of the Green's function. Our proof for the convergence of the expansion for $u_h - u_{h,d}$ is based on uniform $W^{1,\infty}$ estimates on the potential u_h of the reference network and on the corresponding discrete Green's function. These estimates are derived using the periocity of the reference network and the 3 step compactness method of A. Avellaneda and F.H. Lin (Comm. Pure Appl. Math., 40, pp. 803-847, 1987). Work done in collaboration with Sivaji Ganesh Sista.

A hierarchical structural and material optimization model for bone-remodelling simulation. **Helder Rodrigues** (Universidade Técnica de Lisboa, Portugal), Pedro Coelho (Universidade Nova de Lisboa, Portugal), Paulo Fernandes (IDMEC-IST, Portugal) IC/MT2446/015

Bone is a natural cellular material that is in a permanent process of remodeling. The bone remodeling depends on biological and mechanical factors. This work describes a computational model where the law of bone remodeling is derived assuming that bone adapts in order to achieve the stiffest structure for given load conditions while the total amount of bone mass is regulated by a global constraint quantifying the biological factors . Here bone is assumed to be a non homogeneous cellular periodic material characterized locally by a material unit cell that can vary from point to point. The model assumes two scales for the problem: The global scale (structural or macro scale) where bone is assumed as a continuum material characterized by equivalent (homogenized) mechanical properties. And a local scale (material or micro scale) where the material unit cell and the respective trabecular structure are defined. At the global scale the problem is to find the bone apparent density distribution and its equivalent material properties. On the other hand and simultaneously, at a local scale the objective is to identify the optimal unit cell characterizing the cellular material. Such model allows the simulation of the remodeling process at two different but interrelated levels, bridging the fundamental scales present (hierarchical). Numerical examples show that bone apparent density and material symmetry distributions are comparable to real bone indicating that bone is actually subjected to an adaptation process that can be modeled with an optimization criterion. However, when the goal is to obtain specific properties of trabecular architecture it is concluded that stiffness is a poor criterion and biological constraints should be carefully considered for a better representation of the bone remodeling process.

IC/MP617/015: Microstructures, PDE and applications. #2

Organiser: Robert Lipton (Louisiana State University, USA)
Co-organiser: Alain Damlamian (Université Paris XII, France)

(For abstract, see session #1 above.)

Numerical boundary corrector for elliptic equations with rapidly-oscillating coefficients and new regularity results. **Marcus Sarkis** (WPI/USA and IMPA/Brazil), Henrique Versieux (Courant Institute of Mathematical Sciences, USA) IC/MT2587/015

We introduce and analyze a numerical discretization for a second-order elliptic equation with rapidly oscillating coefficients. The major goal is in the development of a finite element scheme on a mesh size much larger than the scale of the oscillating coefficients and still capturing the oscillations of the solution. The proposed numerical method is based on homogenization theory, and on hybrid finite element methods to treat the boundary corrector term. On the talk we discuss new results on the regularity of the solution of the PDE and on optimal discretization errors. We stress cases where very mild regularity is assumed on the coefficient and so applications to composite materials can be acomplished. Numerical results are presented.

The unfolding approach for the Neumann sieve and other 'strange terms' in periodic homogenization. **Alain Damlamian** (Université Paris XII, France) IC/MT2627/015

We present an extension of the periodic unfolding method which is suited for boundary layers as well as interior layers or "bulk layers", in a periodic setting. As an example, we show how it applies to obtain the "strange term" for periodic homogenization with small Dirichlet holes, as well as to obtain the limit equations for the Neumann Sieve.

A 0-Laplacian approach to impedance imaging. **Yves Capdeboscq** (Université de Versailles St-Quentin, France) IC/MT2674/015

Impedance imaging uses measurements of boundary voltage potentials and associated boundary currents to obtain informations about the internal conductivity profile of an object. Without any *a priori* assumptions about the conductivity profile, impedance imaging is known to be extremely ill-conditioned. The conditioning may be drastically improved in several practical important cases, one such case is that of a known background medium with low volume fraction inhomogeneities. In such a case, the first order perturbation induced by the inhomogeneities appears by the mean of a polarization tensor.

The subject of this talk is to show that such a tool can also be used for the determination of a global conductivity profile of an arbitrary object, provided that the electric measurements are coupled with elastograhic data.

The underlying non-linear partial differential equation to be solved is of the form

$$\operatorname{div}\left(a(x)\frac{\nabla u}{|\nabla u|^2}\right) = 0,$$

which can be interpreted as a 0- Laplacian. We will show that this equation can be successfully solved to recover the conductivity map.

This work is a collaboration with H. Ammari and E. Bonnetier.

Local-field assessment inside multi-scale composite microstructures. **Timothy Breitzman** (Universal Technology Corporation, USA), Robert Lipton (Louisiana State University, USA), Endel Iarve (University of Dayton Research Institute, USA) IC/MT3352/015

We introduce a new rigorous asymptotic theory for recovering the local field behavior inside multi-scale prestressed composite micro-structures. The theory applies to zones containing abrupt changes in the composite microgeometry. This includes the interfaces between plies inside fiber reinforced laminates. The asymptotic expansions are used to develop a fast numerical algorithm to extract local field information inside a prescribed subdomain without having to resort to a full numerical simulation. For regions of homogeneous microstructure, the analysis delivers rigorous upper bounds on the magnitude of the local stress and strain fields inside the composite. Numerical examples are provided to demonstrate the utility of the new asymptotic theory for quickly assessing the location and magnitude of local field concentrations inside complex multi-scale composite microstructures

IC/MP335/015: Mathematical challenges in the geosciences.

Organiser: Carsten Mayer (TU Kaiserslautern, Germany)

During the last years technological progress has changed the observational methods in all fields of geosciences completely. Modern satellite based techniques are entering geoscientific fields like geophysics, geodesy, meteorology and many others. The increasing flow of data of very high accuracy demands adequate mathematical tools to solve the geoscientific problems. Techniques from fields like constructive approximation, differential and integral equations, potential theory and many more have to be developed in order to assess the data and to build an objective basis for scientific solution of geoscientific problems.

Locally-supported spherical wavelets based on block grids. **Michael Schreiner** (Neu-Technikum Buchs, Switzerland) IC/MT1897/015

We present a method for approximating spherical functions from discrete data on a block grid structure. The essential ingredients of the approach are scaling and wavelet functions within a biorthogonalisation process generated by locally supported zonal kernel functions. In consequence, problems involving rotation–invariant pseudodifferential operators become attackable. A multiresolution analysis is formulated enabling a fast wavelet transform similar to the algorithms known from one–dimensional Euclidean theory.

Slepian functions on the sphere: problems, solutions, challenges. **Frederik Simons** (Princeton University, USA), F Dahlen (Princeton University, USA), Mark Wieczorek (IPG Paris, France) IC/MT1142/015

I will review the properties of spherical Slepian functions and discuss their meritorious applicability in the Earth and space sciences. In a 2006 SIAM Review paper, we named "Slepian functions" those linear combinations of surface spherical harmonics that, while bandlimited, are optimally concentrated in a surface spatial domain of arbitrary description, or, alternatively, those that are strictly spacelimited but optimally concentrated in the spectral domain. They are eigenfunctions of a "spatiospectral concentration kernel", the spherical analogue of an operator first studied by David Slepian, in one and two, and later by Alberto Grunbaum, in higher dimensions. If the region of concentration is an axisymmetric polar cap, or an (also equatorially symmetric) double polar cap, the spherical Slepian matrix concentration operator commutes with a simple tridiagonal matrix that has analytically prescribed elements, and their eigenfunctions, the (spherical harmonic expansion coefficients of) Slepian functions are found easily and with great stability. For applications in the Earth sciences, the spatial concentration domain would be a geologically relevant domain (Belgium or all of the World's oceans), in which case the concentration operator may be found by numerical integration. Slepian functions are not wavelets, but they are self-similar in an asymptotic limit of large bandwidths and small concentration areas. We may use them to calculate local spatial contributions to the global spherical harmonic spectrum of geophysical fields, such as Earth or planetary gravity, topography or their correlation. They are useful to compute global spherical harmonic expansions and spectra of fields observed over incomplete domains, such as Earth or planetary magnetic fields, which typically are unobserved over small polar caps, or, farther out in the solar system, to compute the cosmic microwave background spectrum from observations masked by strong emissions from the galactic plane.

Efficient reconstruction of functions on the sphere from scattered data. **Daniel Potts** (TU Chemnitz, Germany), Jens Keiner (Universität Lübeck, Germany), Stefan Kunis (TU Chemnitz, Germany) IC/MT3434/015

Recently, fast and reliable algorithms for the evaluation of spherical harmonic expansions have been developed. The corresponding sampling problem is the computation of Fourier coefficients of a function from sampled values at scattered nodes. We consider a least squares approximation as well as an interpolation to the given data. Our main result is that the rate of convergence of the two proposed iterative schemes depends only on the mesh norm and the separation distance of the nodes. In conjunction with the nonequispaced FFT on the sphere, the reconstruction of N^2 Fourier coefficients from M reasonably distributed samples is shown to take $\mathcal{O}(N^2 \log^2 N + M)$ floating point operations. Numerical results support our theoretical findings.

From the sphere to more realistic geometries. **Willi Freeden** (TU Kaiserslautern, Germany) IC/MT1831/015

The Earth is an almost perfect sphere. This is the reason why the foundation of my Geomathematics Group Kaiserslautern (in 1994) was meant to improve spherical(ly oriented) tools (such as splines, wavelets etc), e.g., in gravitation, magnetics, hydrodynamics, solid body sciences. The dramatic change in the observational situation caused by modern (satellite) instruments during the last years, however, requires new components of mathematical thinking and adapted strategies to obtain high-precision solutions. In consequence, there is an increasing need for mathematical research observing the non-sphericity of the Earth. The lecture presents recent geomathematical developments on geoscientifically relevant geometries such as ellipsoid, geoid, (actual) Earth's surface, and (real) 'surfaces' of (low) Earth's orbiters.

IC/MP335/015: Mathematical challenges in the geosciences. #2

Organiser: Carsten Mayer (TU Kaiserslautern, Germany)

(For abstract, see session #1 above.)

Wavelets and splines for modelling the earth's magnetic field. **Carsten Mayer** (TU Kaiserslautern, Germany) IC/MT3444/015

At the present time there is an unprecedented opportunity to use satellite magnetometer data, as for example Oersted and CHAMP records, to improve our knowledge of the Earth's magnetic field and its sources. These measurements contain contributions from the main magnetic field of the Earth, the crustal field as well as contributions coming from different exterior (ionospheric and magnetospheric) sources. For the mathematical analysis of the data it is critical to have in hand appropriate tools which separate these sources and which are able to analyze the different contributions independently.

We will present in this talk an approach in terms of (spherical) scalar and vectorial scaling functions and wavelets to handle these problems. Examples include crustal field modelling and reconstruction of ionospheric currents. At the end we will present an approach by vectorial splines defined in the exterior of a sphere, which seam to be more appropriate to handle measurements on realistic satellite orbits.

Modeling of potential fields with wavelet frames. **Matthias Holschneider** (Universität Potsdam, Germany) IC/MT2277/015

We investigate the numerical challenges associated with the modelling of geophysical potential fields with the help of frames. Special emphasis is put to the construction and application of frames of Poisson wavelets.

Using multi-point measurements to investigate waves in the earth's magnetosphere. **Dragoş Constantinescu** (TU Braunschweig, Germany), Karl-Heinz Glassmeier (TU Braunschweig, Germany), Yasuhito Narita (TU Braunschweig, Germany) IC/MT1464/015

Multi-point measurements in the extraterrestrial space have been routinely available only after the launch of the CLUSTER spacecraft fleet at the end of year 2000. Unlike the sensor arrays commonly used in related fields of geosciences, CLUSTER offers only a minimal set of four sensors placed in a tetrahedron configuration. To take advantage of the full potential of these measurements, advanced tools from seismology have been adapted to be used with magnetized plasma waves. One class of these tools uses a minimization technique to decompose the measured wave field into elementary wave components. We present the formalism and application of two of these tools: The *wave telescope* which corresponds to plane waves decomposition, and the *source locator* which corresponds to spherical waves decomposition. For a given frequency they provide either the wave vector or the wave length and the source position, respectively. Using CLUSTER magnetic field measurements it is possible to determine wave propagation directions, dispersion relations, and spatial distribution and motion of the plasma wave sources.

Using non-linear MOS techniques for forecasting global radiation from MSG satellite data. **Martin Fengler** (Meteomedia AG, Switzerland) IC/MT3079/015

For more than 30 years Model Output Statistics (MOS) have been well known to meteorologists. MOS techniques are used for a statistical post-processing of the Direct Model Output (DMO) obtained by numerical weather prediction codes. The success of a MOS system based on classical linear regression originates from ŞlearningŤ a statistical relationship between the weather forecasting model and the local environment of the weather station, e.g. effects in the boundary layer which are not modelled by DMO such as fog, luv- and lee effects, as well as shadow in mountainous terrain. While MOS benefits from a good numerical weather prediction code, it is able to reduce the forecast error for so called point forecasts significantly: For example, depending on the location the mean absolute error in temperature can be decreased from 3-4 K to 0.6-1 K for a day ahead forecast. However, from a mathematical point of view linear regression is for most weather parameters, for example, such as precipitation, wind, radiation, and cloud cover not a suitable approximation method since these predictands are singly or doubly truncated, which is not reflected by the linear model. In this talk we propose non-linear approximation techniques that solve this problem and demonstrate their application to global radiation data obtained from MSG satellite data.

IC/MP183/015: Trends in tomography.

Organiser: Eric Todd Quinto (Tufts University, USA)
Co-organiser: Adel Faridani (Oregon State University, USA)
Co-organiser: Andreas Rieder (Universität Karlsruhe, Germany)

Tomography consists of a broad range of applied mathematics and technologies that are important for medicine and industry, and this minisymposium will feature some of the newest and most exciting developments. Seminal work in several areas will be represented including new methods in three-dimensional tomography including dynamic tomography and sampling, new applications of local tomography to electron microscopy, and thermoacoustic tomography. Combining tomographic reconstruction and post-processing promises to provide better diagnostic information and we will invite speakers to give the latest developments in this area. New algorithms for dynamic CT promise to show heart movement, and researchers will present their latest work. Thermoacoustic tomography is an exciting new field that combines important pure mathematics, the spherical Radon transform, with applications to diagnostic medicine, and in particular cancer detection.

Ultrasound attenuation in thermo-acoustic tomography. **Sarah Patch** (University of Wisconsin, Milwaukee, USA) IC/MT1326/015

Idealized thermo/photo/opto-acoustic (TPOAT) data are unattenuated acoustic pressure measurements, representing spherical integrals of an internal acoustic source. Inversion formulae already exist for idealized data in several different measurement geometries. However, ultrasound pulses attenuate as they travel through biological tissue, degrading reconstructed image quality. Widely accepted accepted models of ultrasound attenuation contradict the widely accepted paradigm of constant and *finite* propagation speed. Different explanations for this paradox will be discussed.

Photo-acoustic tomography with integrating line detectors and the circular Radon transform. **Markus Haltmeier** (Universität Innsbruck, Austria), Robert Nuster (Universität Graz, Austria) IC/MT2757/015

Photoacoustic (or thermoacoustic) tomography is an emerging hybrid imaging method for non-invasive medical diagnosis and fully three-dimensional visualization of biological probes. Within this modality electromagnetic illumination is used to induce acoustic waves inside an object of interest. In this talk we assume that a cylindrical array of line detectors is used to record the acoustical data. This leads to the mathematical problem of inverting the circular Radon transform (or equivalently reconstructing a function from its integrals over certain circles). The circular Radon transform arises in several other up-to-date imaging modalities, such as RADAR imaging or ultrasound tomography.

In this talk we present a stable formula (based on series expansions) for recovering a planar function from its circular Radon transform. We apply this formula to obtain an exact three imaging algorithm for photoacoustic tomography. We present numerical reconstructions with real and synthetic data.

A parametric level-set approach to tomographic reconstruction. **Misha Kilmer** (Tufts University, USA) IC/MT2765/015

A common problem in tomographic imaging is the reconstruction of one or more oddly shaped regions of interest, or hot spots, distinct from the background. In diffuse optical tomography for breast tissue imaging, for example, the goal is to recover 3D images of absorption and diffusion of light in tissue with anomalous regions of high absorption and diffusion indicating the presence of cancer. Unfortunately, many tomographic reconstruction problems are severely underdetermined if each voxel value is independently considered to be an unknown. Furthermore, noise in the measured data makes reconstruction of useful images virtually impossible. We propose a model for the underlying images of interest which makes the problem much better determined, thus improving the computational complexity to the problem, and which helps to address the sensitivity to noise. In particular, we introduce a general formulation of a level-set description of the space-varying perturbation defined through a linear combination of basis functions. Our approach is different from traditional level set approaches in that the inverse problem requires only the reconstruction of the expansion coefficients in the basis, as well as a few auxiliary parameters describing the background and intensity of the anomaly(ies). In this way, we are able to ensure some degree of regularization through the model itself. We present computational results that show the promise of our approach.

This is joint work with Ashley B. Tarokh and Eric Miller

Parameter and structure identification in optical tomography. **Simon Arridge** (University College London, UK) IC/MT2920/015

Optical Tomography is an emerging medical imaging modality that is relatively cheap, fast, and offers a contrast mechanism that is complementary to other modalities such as Magnetic Resonance Imaging. From the mathematical point of view the inverse problem is non-linear and illposed, and is commonly treated as a parameter identification problem for the coefficients of a numerical method such as the finite element method (FEM), typically represented in a local pixel basis. Alternatively, shape based methods, either implicit (such as level sets) or explicit (via a parametric surface model) can be used to identify *structures* . In this talk I will present some recent results comparing these approaches.

IC/MP183/015: Trends in tomography. #2

Organiser: Eric Todd Quinto (Tufts University, USA)
Co-organiser: Adel Faridani (Oregon State University, USA)
Co-organiser: Andreas Rieder (Universität Karlsruhe, Germany)

(For abstract, see session #1 above.)

Cone beam CT: reconstruction formulas and resolution. **Alfred Louis** (Universität des Saarlandes, Germany) IC/MT2356/015

In cone beam CT the mathematical model is described by the integral transform

$$Df(a,\theta) = \int_0^\infty f(a+t\theta)dt$$

where $a \in \Gamma$ is a source position and $\theta \in S^2$ are the direction of the rays. For curves Γ satisfying the Tuy–Kirillov condition we derive inversion formulas based on the approximate inverse. To this end we study invariances of the operator depending on the curve Γ. If the Tuy–Kirillov condition is not fulfilled we give approximations, and especially for the classical circular scanning geometry we present explicit representations of the reconstruction kernel.

The resolution is studied based on the singular value decomposition for the operator derived from the classical SVD for the Radon and the parallel beam x-ray transform. Applications to x-ray CT and to phase contrast tomography are discussed.

Application of microlocal analysis to electron tomography. **Ozan Öktem** (Sidec Technologies, Sweden), Eric Todd Quinto (Tufts University, USA) IC/MT2018/015

We will begin with a very brief overview of electron tomography from an integral geometric viewpoint with a particular emphasis on the role of the filtered backprojection algorithm. Next, we touch upon a number of difficulties that arise in electron tomography, namely the high degree of clutter, the extremely low signal-to-noise ratio in the data, and the limited data problems that lead to severe ill-posedness. We then present a new local tomographic algorithm applicable to electron tomography and using microlocal analysis, we characterize those singularities that are stably visible from the limited data given by the data collection protocol in the electron microscope. In conjunction with this we also mention some open problems, in particular the problem of defining a concept of resolution. Finally, if time permits, we provide reconstructions from both real and simulated electron tomography data.

Accurate reconstruction of functional and geometric parameters in tomography. **Ronny Ramlau** (RICAM Linz, Austria) IC/MT1837/015

In some medical applications, e.g. for the planning of a surgery, it is necessary to determine the accurate boundary of inner organs. Usually this is done in two steps: First, the density distribution is reconstructed from a CT scan. In a second step the jumps in the reconstruction are determined by image processing methods. In our talk, we propose a variational method that allows to reconstruct both the functional parameters (the density distribution) and the geometric parameters (the discontinuity set). We will restrict ourselfs to the reconstruction of piecewise constant or piecewise smooth functions. The reconstructions will be obtained by the minimization of a Mumford - Shah type functional. We will present analytical results for Computerized Tomography as well as Single Photon Emission Computed Tomography (SPECT). In particular, a regularization theory for our method will be developed. We will give numerical results for both applications and will also consider the limited angle case.

This talk is joint work with Wolfgang Ring (University of Graz, Autria) and Esther Klann (Radon Institute, Linz, Austria).

Current problems in vector and tensor tomography. **Thomas Schuster** (Universität Hamburg, Germany) IC/MT1522/015

Vector and tensor tomography deal with the reconstruction of a tensor field $f = f_{i_1 \dots i_m}$ from observations $\Phi(f)$. Applications can be found in medical imaging, photoelasticity, nondestructive testing, plasma physics or problems connected with electro magnetism. Over the last years not only the areas of applications for that kind of tomography has grown but also the number of approaches for solving the different inverse problems $\Phi(f) \mapsto f$. In this talk we want to give an impression of some tensor tomography problems which are currently under investigation. One important example for a mapping Φ is

given by the cone beam ray transform for tensor fields

$$\mathbf{D}f(\alpha,\omega) = \int_0^\infty \langle f(\alpha+t\omega),\omega^m\rangle\,\mathrm{d}t\,,$$

where $\alpha \in \Gamma$ denotes the source of the beam and $\omega \in S^{n-1}$ is a vector of direction. For $m = 1$ this transform is known as Doppler transform and represents the mathematical model in Doppler tomography. In the talk we present ideas for the inversion of $\mathbf{D}$ with the help of the method of approximate inverse as well as a generalization of the known formula of Grangeat for arbitrary rank m. Some numerical results for the parallel geometry are presented as well. As a relatively new field of tensor tomography concerning tensors of rank 2 we further introduce to the problem of polarization tomolgraphy. Here, the aim is to recover the anisotropic part χ of the permeability tensor $\varepsilon_{ij} = \varepsilon\delta_{ij} + k^{-1}\chi_{ij}$ with the help of Rytow's law:

$$\frac{D\eta}{d\tau} = \frac{i}{2n^2}P_{\dot\gamma}\chi\eta\,.$$

The most general setting of the problem is to determine χ from the linear mapping $U(\gamma)$ satisfying $\eta(1) = U(\gamma)\eta(0)$. We present a uniqueness result for the linearized problem which was obtained by Sharafutdinov. A numerical solver for this highly demanding tomographic problem is still searched.

IC/MP342/015: Bregman distances in optimization, inverse problems and financial mathematics.

Organiser: Elena Resmerita (RICAM Linz, Austria)
Co-organiser: Hansjoerg Albrecher (RICAM Linz, Austria)

Bregman distances associated with convex functions were introduced in the sixties as tools for approaching optimization problems, although particular forms, such as the Kullback-Leibler distance, had been used in information theory and statistics about a decade earlier. Since then, generalized distances have been employed when designing and/or analyzing methods for solving problems from optimization, statistics, inverse problems and, more recently, financial mathematics, machine learning, etc. Nowadays, the interest in using Bregman distances is growing in most of these fields, due to a cross-over effect: new results related to Bregman distances reported in a field have stimulated investigations in others.

The aim of this symposium is an interdisciplinary exchange of research ideas based on the common denominator provided by Bregman distances. The speakers cover some of the many areas which have benefited over the years from the use of Bregman distances. These distances and associated projections have been employed towards the solution of nonlinear operator equations and variational inequalities. In ill-posed inverse problems, such as those encountered in image denoising, Bregman distances have been successfully exploited in various regularization procedures. In mathematical finance, Bregman distances have been used for efficient calibration algorithms of volatility surfaces as well as to determine suitable pricing measures in incomplete markets, for instance in approximation schemes for the arbitrage-free equilibrium pricing measure.

A perspective on Bregman distances, Bregman projections and their applications. **Elena Resmerita** (RICAM Linz, Austria), Dan Butnariu (University of Haifa, Israel) IC/MT515/015

The concepts of Bregman distance and Bregman projection originate in a 1967 work of Lev Bregman. Since then, the use of these concepts became integral part of contemporary convex analysis, leading to a new theoretical paradigm, and to powerful techniques of solving optimization problems, operatorial equations and variational inequalities. The aim of this talk is to presents, in a coherent perspective, basic notions, theoretical results and potential applications which emerged from the study of Bregman distances and Bregman projections. We will touch notions like Legendre function, totally convex function, their inter-relations and connections with the geometry of the spaces in which they are living. We will show how such notions and connections became tools in the build up of algorithms for convex optimization and for other purposes. Also, we will point out some actual and potential applications of those algorithms.

Error estimation in TV imaging. **Martin Burger** (Universität Münster, Germany), Elena Resmerita (RICAM Linz, Austria), Stanley Osher (University of California, Los Angeles, USA) IC/MT628/015

Total variation based methods are popular in image processing due to their cartoon extraction capabilities. Concerning their analysis schemes based on total variation minimization pose various challenging problems caused by the arising degeneracies and strong nonlinearities.
In this talk we will highlight how Bregman distances related to the total variation seminorm can be used to perform error estimation for several total variation based schemes such as the classical ROF model of image processing, iterative refinement, and inverse scale space methods. Moreover, we shall also discuss the use of Bregman distances for the numerical analysis of discretization schemes.

On pricing derivatives under GARCH models: a dynamic Gerber-Shiu's approach. **Hailiang Yang** (University of Hong Kong) IC/MT1284/015

This paper proposes a method for pricing derivatives under the GARCH assumption for underlying assets in the context of a "dynamic" version of Gerber-Shiu's option-pricing model. Instead of adopting the notion of local risk-neutral valuation relationship (LRNVR) introduced by Duan (1995), we employ the concept of conditional Esscher Transforms introduced by Bühlmann et al. (1996) to identify a martingale measure under the incomplete market setting. One advantage of our model is that it provides a unified and convenient approach to deal with different parametric models for the innovation of the GARCH stock-price process. Under the conditional normality assumption for the stock innovation, our pricing result is consistent with that of Duan (1995). In line with the celebrated Gerber-Shiu's option pricing model, we can justify the pricing result within the dynamic framework of utility maximization problems which makes the economic intuition of the pricing result more appealing. In fact, the use of the Esscher Transform for option valuation can also be justified by the minimization of the relative entropy between the statistical probability and the risk-neutralized pricing probability. Numerical results for the comparison of our model with the Black-Scholes option pricing model are presented.

Generalized Kullback-Leibler distances for some optimal financial decisions. **Wolfgang Stummer** (Universität Erlangen-Nürnberg, Germany) IC/MT3864/015

We study Bayesian decision making based on observations of the price dynamics $(X_t : t \in [0,T])$ of a financial asset, when the hypothesis model is a diffusion process with time-dependent volatility and price-dependent drift, and the alternative model is another diffusion process with the same volatility but with different drift.

The presented methods are fundamentally based on investigations about the time-behaviour of power divergences (which are generalizations of the well-known Kullback-Leibler(-Bregman-) distance) between the hypothesis model and the alternative model.

We obtain exact formulae and bounds (in terms of the observation duration T) of the corresponding minimal mean decision loss (Bayes risk, Bayes loss), and the associated decision risk reduction.

We will also show some convergence results for corresponding discrete-time approximations, as well as effects on the non-commutativity between Bayesian statistical and optimal investment decisions.

IC/MP4057/015: Compressed sensing II: algorithms and applications.

Organiser: Justin Romberg (Georgia Institute of Technology, USA)
Co-organiser: Robert Nowak (University of Wisconsin, Madison, USA)
Co-organiser: Jared Tanner (University of Utah, USA)

This minisymposium complements the main Compressed Sensing (CS) one by concentrating on applications of the theory. It includes researchers interested in practical optimization algorithms for recovery from limited measurements, and those developing novel imaging devices based on the methods of CS.

Due to the nascent state of Compressed Sensing, it is particularly important that theoretical researchers interact with those interested in applications. Both the theoreticians and the practitioners will benefit from this interaction. Many practical aspects of algorithms and devices have been influenced by theoretical ideas. Application researchers have begun to see what is and is not practical within the CS framework, and in the process have uncovered interesting mathematical problems.

Compressive imaging. **Justin Romberg** (Georgia Institute of Technology, USA) IC/MT3415/015

We will discuss Compressed Sensing in the context of practical image recovery. Our first topic will be the extension of the CS theory from random measurements to bounds for general measurement/sparsity pairs. Next, we will discus image models that "go beyond ℓ_1", showing how ideas from variational image processing can naturally be incorporated into the CS framework. Finally, we will talk about algorithmic techniques for solving the large-scale optimization problems we encounter in CS.

Task-specific compressive sensing with a multiplexing hyperspectral imager. **Robert Muise** (Lockheed Martin Corporation, USA) IC/MT3476/015

In Task-Specific compressive sensing, the goal is to integrate the sensing process with the final exploitation task in a way that significantly reduces the sensing measurements which would normally be required to reconstruct the entire full resolution scene. We present an algorithm which incorporates a pattern recognition metric into the sensing process. The interaction between the sensing and the exploitation algorithms result in the collection of a variable resolution scene where full resolution is collected only where it is required by the exploitation algorithm. We demonstrate this Task-Specific compressed sensing system utilizes a near Infrared (NIR) Hadamard multiplexing imaging sensor. This prototype sensor incorporates a digital mirror array (DMA) device in order to realize a Hadamard multiplexed imaging system. Specific Hadamard codes can be sent to the sensor to realize inner products of the underlying scene rather than the scene itself. The developed sensing algorithm incorporates the exploitation tasks into the sensing by computing a pattern recognition metric which directs the sensor to collect only the information relevant to the recognition problem. The result is a multiple resolution hyperspectral cube with full resolution where patterns are present and less than full resolution where there are no patterns of interest. We demonstrate this algorithm fully integrated with the sensor and running in real time on a test case to demonstrate feasibility.

Compressive signal processing. **Richard Baraniuk** (Rice University, USA) IC/MT3714/015

Despite the apparent need for adaptive, nonlinear techniques for dimensionality reduction, random linear projections have proven to be extremely effective at capturing signal structure in cases where the signal obeys a low-dimensional model. Similarly, random projections are a useful tool for solving problems where the ultimate question of interest about the data requires a small amount of information compared to the dimensionality of the data itself. The success of random projections in both of these arenas can be traced to an elementary concentration of measure property, which allows us to extend the utility of random projections to a variety of new signal models and applications.

This is joint work with Mark Davenport and Mike Wakin.

The surprising structure of Gaussian point-clouds and its implications for signal processing. **Jared Tanner** (University of Utah, USA), David Donoho (Stanford University, USA) IC/MT3478/015

We will explore connections between the structure of high-dimensional convex polytopes and information acquisition for compressible signals. A classical result in the field of convex polytopes is that if N points are distributed Gaussian iid at random in dimension $n << N$, then only order $(\log N)^n$ of the points are vertices of their convex hull. Recent results show that provided n grows slowly with N, then with high probability all of the points are vertices of its convex hull. More surprisingly, a rich "neighborliness" structure emerges in the faces of the convex hull. One implication of this phenomenon is that an $N-$vector with k non-zeros can be recovered computationally efficiently from only n random projections with $n = 2ek\log(N/n)$. Alternatively, the best $k-$term approximation of a signal in any basis can be recovered from $2ek\log(N/n)$ non-adaptive measurements, which is within a log factor of the optimal rate achievable for adaptive sampling. Additional implications for randomized error correcting codes will be presented.

This work was joint with David L. Donoho.

IC/MP178/015: Compressed sensing.

Organiser: Justin Romberg (Georgia Institute of Technology, USA)
Co-organiser: Robert Nowak (University of Wisconsin, Madison, USA)
Co-organiser: Jared Tanner (University of Utah, USA)

Reconstructing a signal or image from a series of indirect measurements is a fundamental task in the applied sciences. In many applications, the acquisition process can be mathematically modeled as a (known) linear operator applied to an unknown signal or image. There are three central questions:

1. How many measurements are needed in order to produce a faithful reconstruction of the signal/image?
2. How is this reconstruction performed?
3. If there is some control over the measurement process, then what is the best acquisition strategy (linear operator) to use?

The nascent field of Compressed Sensing (CS) addresses these questions using the machinery of computational harmonic analysis. The central results, which have appeared very recently, state that for an appropriate measurement system the number of measurements required to reconstruct an image depends on the *inherent complexity* of the image, rather than the desired resolution of the reconstruction. Numerous algorithms have been recently proposed to perform this reconstruction, drawing on ideas from convex optimization, model selection in statistics, and spectrum estimation in signal processing.

The implications of this newfound theory are widespread. Essentially, it tells us that the number of measurements we need to create high-quality images is far less than the classical Nyquist–Shannon theory suggests. As a consequence, acquisition time can be reduced substantially by committing computational resources to the reconstruction. In addition, the CS suggests new *universal* measurement schemes; non-adaptive linear operators that can be used to reconstruct many different classes of signals.

An information-theoretic view of compressive sampling. **Vivek Goyal** (Massachusetts Institute of Technology, USA), Alyson Fletcher (UC Berkeley, USA), Sundeep Rangan (QUALCOMM Flarion Technologies, USA) IC/MT3526/015

Encouraging recent results in compressed sensing or compressive sampling suggest that a set of inner products with random measurement vectors forms a good representation of a source vector that is known to be sparse in some fixed basis. With quantization of these inner products, the encoding can be considered universal for sparse signals with known sparsity level. We analyze the operational rate-distortion performance of such source coding both with genie-aided knowledge of the sparsity pattern and maximum likelihood estimation of the sparsity pattern. We show that random measurements induce an additive logarithmic rate penalty, i.e., at high rates the performance with rate $R + O(\log R)$ and random measurements is equal to the performance with rate R and deterministic measurements matched to the source.

Compressed sensing and best k-term approximation. **Albert Cohen** (Université Paris VI, France) IC/MT3730/015

In this talk, we shall review several recent results revolving around how well compressed sensing can approximate a given signal from a prescribed budget of linear measurements, as compared to adaptive nonlinear measurements. It will be shown that the answer to this question heavily depends on the norm in which the error is measured, and can be understood through the analysis of the null space of the compressed sensing matrix.

Sampling parametric non-bandlimited signals. **Martin Vetterli** (École Polytechnique Fédérale de Lausanne, Switzerland), Pier Luigi Dragotti (Imperial College London, UK) IC/MT3802/015

Consider the problem of sampling signals which are not bandlimited, but still have a finite number of degrees of freedom per unit of time, such as, for example, piecewise polynomials. Call the number of degrees of freedom per unit of time the rate of innovation. We demonstrate that by using an adequate sampling kernel and a sampling rate greater or equal to the rate of innovation, one can uniquely reconstruct such signals. We thus prove theorems for classes of signals and sampling kernels that generalize the classic "bandlimited and sinc kernel" case. In particular, we show sampling theorems for periodic as well as finite length piecewise polynomials, using a bandlimited derivative kernel, as well as a Gaussian kernel. For infinite signals with a finite local rate of innovation, we show exact local reconstruction algorithms using a rich class of sampling kernels such as functions satisfying Strang-Fix conditions, Exponential Splines and functions with rational Fourier transform. For the case of piecewise sinusoidal signals, we show that there is a trade-off between the number of sinusoids per piece and the proximity of the discontinuities in order to have perfect reconstruction. We thus put forward a parametric uncertainty principle. We also show some extensions to 2-dimensional signals, as well as methods for dealing with the noisy case. All the results presented lead to computational procedures that are readily implementable, which is shown through experimental results. Applications of these new sampling results can be found in signal processing, communications systems and biological systems. In particular, we will show how these results can be used for ultra-wideband (UWB) communications or for image super-resolution.

Sparse representations using constructive frames. **Vahid Tarokh** (Harvard University, USA) IC/MT4433/015

For the noisy sparse representation problem and any arbitrary frame, we will establish a limit on the trade-offs between dimension, sparsity, redundancy and average distortion. We will then present a class of constructive frames endowed with a real time representation algorithm that can approach these limits.

This presentation is based on joint work with Mehmet Akcakaya.

IC/MP178/015: Compressed sensing. #2

Organiser: Justin Romberg (Georgia Institute of Technology, USA)
Co-organiser: Robert Nowak (University of Wisconsin, Madison, USA)
Co-organiser: Jared Tanner (University of Utah, USA)

(For abstract, see session #1 above.)

Optimized projections for compressed sensing. **Michael Elad** (Technion – Israel Institute of Technology) IC/MT3431/015

Compressed-Sensing (CS) offers a joint compression- and sensing-processes, based on the existence of a sparse representation of the treated signal and a set of projected measurements. Work on CS thus far typically assumes that the projections are drawn at random. In this talk we describe ways to optimize these projections. Two methods are considered: (i) A direct optimization with respect to the CS performance, targeting CS applied with the Orthogonal Matcing Pursuit (OMP), and (ii) A simpler method that targets an average measure of the mutual-coherence of the effective dictionary. Both techniques are demonstrated and shown to lead to better CS reconstruction performance.

The Johnson–Lindenstraus lemma in compressed sensing. **Ronald DeVore** (University of South Carolina, USA) IC/MT3458/015

We shall show that the Johnson-Lindenstrauss lemma, prominent in the geometry of Banach spaces, implies the Restricted Isometry Property for random matrices. The importance of this result is that there are simple proofs of the JL lemma and thus there is a simple avenue to verify the RIP.

Fast Reconstruction Algorithms for Compressed Sensing. **Robert Nowak** (University of Wisconsin, Madison, USA), Steve Wright (University of Wisconsin, USA) IC/MT3731/015

It is possible to reconstruct a signal from a relatively small number of samples, a number proportional to the number of coefficients required in the optimal compression of the signal. Moreover, these key samples need not be adaptive, instead they take the form of randomized projections of the signal. This new form of sampling, known as Compressed Sensing (CS), is causing a dramatic re-thinking of the basic fundamentals of sensing and sampling. This talk will describe new algorithms for CS reconstruction problems.

Beyond Nyquist: efficient sampling of sparse, band-limited signals. **Joel Tropp** (The University of Michigan, USA) IC/MT3495/015

The standard approach to measuring a bandlimited signal requires samples at the Nyquist rate, which is twice the highest frequency present in the signal. For many signals of interest, this sampling rate is beyond the power of current technologies. Fortunately, most signals contain very few significant frequencies relative to their nominal bandwidth. Recent developments in computational harmonic analysis offer the possibility of acquiring these signals using far fewer samples. One architecture that has been proposed involves modulation of the signal by a random square wave, followed by low-pass filtering and low-rate sampling. This talk describes methods for analyzing this system mathematically. The results establish that the random modulator collects enough information to reconstruct frequency-sparse signals. There are also surprising implications for the implementation of the system.

IC/MP73/054: Wavelet methods for real-world problems.

Organiser: Abul Hasan Siddiqi (King Fahd University, Saudi Arabia)

Wavelet and Gabor analysis have attracted the attention of researchers in different parts of the world belonging to different areas of human knowledge in the recent past. Wavelet packets and Wave packets are comparatively new genralizations of wavelet and Gabor systems. The basic properties of these two systems are being investigated. In the present symposium besides applications of wavelet methods to climatology and finance, fundamental properties of these two new systems will be discussed.

Oil exploration and wavelet microscope. **Abul Hasan Siddiqi** (King Fahd University, Saudi Arabia) IC/MT4978/054

Wavelet analysis is a refinement of Fourier analysis. Its applications to various disciplines such as signal analysis and image processing, meteorology, bioinformatics, pattern recognition, cardiology, scientific computing, financial engineering and stratigraphy have been studied in the recent years. There is a close connection with the Milankovitch theory of climatic change and sedimentary cycles of certain regions of the world.

Definition and interpretation of sedimentary facies often involves examination of well logs to assess values, trends, cycles, and abrupt changes. The procedure, which is often visual inspection of the logs (well logging is a technique used in oil and gas industry for recording rock and fluid properties to find hydrocarbon zones in the geological formations within Earth's crust), could be improved by using recently developed signal analysis and features extraction techniques based on wavelet analysis. In particular, wavelet analysis of logs provides an early interpretable visual representation of signals and is an efficient tool for supporting stratigraphic analysis (stratigraphy is a branch of geology dealing essentially with the study of rock layers and layering. It is mainly used in the study of sedimentary and layered volcanic rocks). Wavelet methodology permits the detection of cyclicities, trends and sudden changes in sedimentary successions. The speaker and his coworkers have tested wavelet methodology for the well logs of an oil field in the Middle East.

Detection of sedimentary cyclicity and stratigraphic completeness by wavelet analysis. **Pammy Manchanda** (Guru Nanak Dev University, India) IC/MT2662/054

On the basis of the time-frequency scaling property of the wavelet transform, accumulation rates and stratigraphic completeness can be calculated for various observation time span by using wavelet analysis. Wavelet analysis also allows automatic detection of high-frequency sedimentary cyclicity and abrupt and gradual variations in sedimentation rate. The preservation of different frequency cycles is strongly dependent on variations of the intensity to noise ratio of the original cycles and accumulation rate through time, as demonstrated by computer models. Application of wavelet analysis will be discussed to detect and correlate periodic-cyclic successions of sediments of oil fields.

Saudi meteorological data analysis through wavelet microscope. **Shafiqu Rehman** (King Fahd University, Saudi Arabia) IC/MT1382/054

Wavelet analysis is a refinement of celebrated Fourier analysis which has played a very vital role in understanding real world problems for more than 200 years. The deficiencies of Fourier methods were realized in forties by some leading scientists of that period. Wavelet analysis has been systematically developed in the last two decades and its applications to diverse fields of human knowledge are being investigated. A plot of wavelet coefficients clearly shows the exact location in time of the discontinuity. Wavelet analysis is capable of revealing aspect of data that other signal analysis techniques, miss, aspects like trends, break down points, discontinuities in higher derivatives and self similarities. Further, because it affords a different view of data than those presented by traditional techniques, wavelet analysis can compress or denoise a signal without appreciable degradation of the original signal. Local features of a signal can be described better with wavelets which have a local extent. The wavelet tools can detect the overall trend of a signal.

The time series of meteorological parameters has so much noise that their overall shape is not visible upon visual inspection. It has been observed in our investigation that trends become more and more readable at decomposition at different scales. The wavelets tools have been used in revealing the trends of the meteorological data time series. If the signal

itself includes sharp changes then successive approximation look less and less similar to the original signal. The present paper deals with the meteorological data visualization such pressure, temperature, relative humidity, rain fall and the wind speed time series of the Kingdom of Saudi Arabia. The analysis in this paper is based on discrete and continuous wavelet transforms. The methodology used in this paper is also applicable to study the problems related to oil exploration.

Analysis of NAO, solar flares and sea level changes. **Z. Can** (Istanbul Aydın University, Turkey), Zafer Aslan (Istanbul Aydın University, Turkey), O. Oguz (Istanbul Aydın University, Turkey) IC/MT3317/054

The Relationship between ENSO with ONI and SL Changes are analyzed to define the role of ELNINO3.4 on sea level variations around Turkey and Indian coasts by using monthly sea level time series at 25 sites. There are positive correlation between SL and ENSO and ONI (Warm and cold episodes based on a threshold of +/- 0.5oC for the Oceanic Niño Index (ONI) based on the 1971-2000 base period. For historical purposes cold and warm episodes are defined when the threshold is met for a minimum of 5 consecutive over-lapping seasons. Different techniques have been used to define El Niño event. The most common ones are the Southern Oscillation Index (SOI) and the Niño regions. The Niño regions refer the SST anomalies in defined parts of the Tropical Pacific. There is sufficient evidence on the relation between time series analysis of Sea Level values and ELNINO indices. In northern coastal part of Turkey, the role of positive effect is high. At the western coastal part of Turkey the relation between ELNINO indices and SL is negative. This relation can also be interpreted by applying 1-D Wavelet and Continuous wavelet packets on data. Cross correlation Maps at regional scale for Turkey and India have been presented.

IC/MP73/054: Wavelet methods for real-world problems. #2

Organiser: Abul Hasan Siddiqi (King Fahd University, Saudi Arabia)

(For abstract, see session #1 above.)

Wavelet analysis in the oil industry. **Aiman Mukheimer** (Prince Sultan University, Saudi Arabia) IC/MT3313/054

In the recent years wavelet and wavelet based multifractal analysis have been applied to study and understand cimatic dynmics of different regions.Recently Siddiqi,Rehman and Abbadi have applied these methods to meteorological data of Saudi Arabia.They have mentioned fairly large number of research papers devoted to applications of wavelet analysis to real world systems.There is a close connection between the Milankovitch theory of climatic change and sedimentary cycles of certain regions.Oil industry is quite dependent on proper understanding of sedimentary facies involving examination and iterpretation of well logs.We discuss here how wavelet analysis is used to asses values,trends,correlation and abrupt changes of parameters such as gamma ray,porosity,density.

Wavelets and deblurring operator in seismic records. **Mohammad El-Gebeily** (King Fahd University, Saudi Arabia) IC/MT2861/054

A fixed point method based on wavelets and the minimization of variation is presented for the identification of the blur operator in seismic records. We assume the knowledge of a blurred record and its original version. From this information the blur operator is identified through wavelet transforms and an iterative fixed point method. Numerical examples will be given to confirm the theoretical findings.

IC/MP568/015: Approximation and analysis on the sphere.

Organiser: Ian Sloan (University of New South Wales, Australia)
Co-organiser: Douglas Hardin (Vanderbilt University, USA)

The 2-dimensional sphere is an important setting for applications in geophysics, quantum physics, particle scattering and other fields, yet it presents many mathematical challenges. Many difficulties arise from the absence (except in the special cases associated with the platonic solids) of regular partitions or regular distributions of points on the sphere. Yet progress is being made. This 2-session minsymposium will present current research on approximation (for example, by polynomials and radial basis fuctions) and related methods for partial differential equations on the sphere, together with properties of minimum energy point distributions, and other problems of discretization.

Sobolev bounds on functions on the sphere, with applications to SBFs. **Holger Wendland** (University of Sussex, UK), Joe Ward (Texas A&M University, USA), Francis Narcowich (Texas A&M University, USA) IC/MT3622/055

In this talk we discuss Sobolev bounds on functions that vanish at scattered points on the n-sphere S^n in $\mathbb{R}^{n+1}$. The Sobolev spaces involved may have fractional as well as integer order. We then apply these results to obtain estimates for continuous and discrete least-squares surface fits via spherical basis functions (SBFs). We also address a stabilization or regularization technique known as *spline smoothing*.

Solving pseudo-differential equations on the sphere. **Kerstin Hesse** (University of New South Wales, Australia), Quoc Thong Le Gia (University of New South Wales, Australia), Ian Sloan (University of New South Wales, Australia) IC/MT1283/054

Many important partial differential equations on the sphere can be considered as pseudo-differential equations. In this talk we consider a class of pseudo-differential equations on the sphere and derive an approximate solution with the help of radial basis function collocation. We present error estimates for the approximate solution to the pseudo-differential equation in a Sobolev space setting. We may also discuss some results on boundary value problems on the sphere. This talk is about joint work in progress with Quoc Thong Le Gia and Ian H. Sloan.

Localized polynomial operators for learning functions on the sphere. **Hrushikesh Mhaskar** (CSU Los Angeles, USA), Quoc Thong Le Gia (University of New South Wales, Australia) IC/MT2557/054

Let $\mathbb{S}^q$ denote the unit sphere in $\mathbb{R}^{q+1}$, and μ be its surface area measure. Given a finite set C of points on the sphere $\mathbb{S}^q$, we discuss algorithms to construct weights w_ξ, $\xi \in C$, such that $\int P d\mu = \sum_\xi w_\xi P(\xi)$ for all spherical polynomials P of degree as high as possible. We illustrate our constructions together with the localization properties of certain polynomial operators with a number of examples.

Spectral approximation of Navier–Stokes equations on the unit sphere. **Quoc Thong Le Gia** (University of New South Wales, Australia), Ian Sloan (University of New South Wales, Australia), Mahadevan Ganesh (Colorado School of Mines, USA) IC/MT1280/054

The Navier–Stokes equations describing the movement of a certain fluid with viscosity ν on the unit sphere are

$$u_t + \nabla_u u - \nu \Delta^* u + \nabla p = f\,, \quad \operatorname{div} u = 0\,, \quad u(0) = u_0\,,$$

in which u is the velocity vector field, Δ^* is the Laplace–Beltrami operator, ∇_u is the covariant derivative with respect to vector u, p is pressure, f is the external force, and u_0 is the initial velocity. In this talk, we discuss the spectral method for approximating the solution of the Navier–Stokes equations on the unit sphere using divergence-free vector spherical harmonics. We estimate the error between the approximate solution and the exact solution when f belongs to a certain Sobolev space or is in the Gevrey regularity class of functions. Numerical simulation of the equation using MATLAB will also be discussed.

IC/MP568/015: Approximation and analysis on the sphere. #2

Organiser: Ian Sloan (University of New South Wales, Australia)
Co-organiser: Douglas Hardin (Vanderbilt University, USA)

(For abstract, see session #1 above.)

Bernstein theorems for SBFs on the n-sphere. **Joe Ward** (Texas A&M University, USA) IC/MT3408/054

Bernstein theorems have been known for years for certain classes of functions such as polynomials or univariate splines. They have proven to be extremely useful in obtaining inverse error estimates. In this talk we will discuss Bernstein theorems for various classes of SBFs on the n-sphere and their role in obtaining inverse error estimates for SBF interpolation in various $L^p(S^n)$ norms.

Divergence-free RBFs on spheres and other surfaces. **Francis Narcowich** (Texas A&M University, USA) IC/MT3570/054

In this talk, we present a new tool, based on radial basis functions (RBFs), for fitting a divergence-free vector field tangent to a two dimensional orientable surface $\mathcal{P} \in \mathbb{R}^3$ to samples of such a field taken at scattered sites on $\mathcal{P}$. In the case where $\mathcal{P}$ is a sphere, there are important physical applications. This is joint work with J. Ward and G. Wright.

Asymptotic results for the weighted best-packing problem on rectifiable sets. **Sergiy Borodachov** (Georgia Institute of Technology, USA), Douglas Hardin (Vanderbilt University, USA), Edward Saff (Vanderbilt University, USA) IC/MT2841/054

Different applications such as computer-aided geometric design require placing a large number of points on a surface according to a given non-uniform distribution. For this reason we consider the following generalization of the best-packing problem. Given a compact set $A \subset \mathbf{R}^{d'}$ and function $w : A \times A \to [0, \infty]$, it is required to find the quantity

$$\delta_N^w(A) := \sup_{x_1,\dots,x_N \in A} \min_{i \neq j} w(x_i, x_j) \left| x_i - x_j \right|. \qquad (1)$$

This problem is the limiting case of the minimum weighted discrete Riesz energy problem. When $w(x, y) \equiv 1$ in (1), we get the best-packing problem.

It is known that for any smooth d-dimensional manifold $A \subset \mathbf{R}^{d'}$ $(d \le d')$

$$\lim_{N\to\infty} \delta_N^1(A) N^{1/d} = C_d \, |A|^{1/d}\,, \qquad (2)$$

where $|\cdot|$ denotes the d-dimensional surface area and C_d is a positive constant independent of A. The limit distribution of optimal configurations as N gets large is uniform. (Constant C_d is related to the largest packing density in $\mathbf{R}^d$ and is known only for $d = 1, 2, 3$ – L.Fejes-Tóth, 1953, T.C. Hales, 2005).

We extend estimate (2) and the distribution result for $A \subset \mathbf{R}^{d'}$ being a d-rectifiable set, i.e. an image of a compact set from $\mathbf{R}^d$ with respect to a Lipschitz mapping. In this case the surface area is replaced by the appropriate normalization of the d-dimensional Hausdorff measure $\mathcal{H}_d$.

We also get an analogue of these results for the quantity (1) with the following assumptions about the weight:

1) w is continuous at a diagonal point (x, x) for $\mathcal{H}_d$-almost all $x \in A$;

2) There are at most finitely many points $a_1, \dots, a_n \in A$ $(n \ge 0)$ such that w has a pole at (a_i, a_i), $i = 1, \dots, n$ (the order of each pole is less than one);

3) For every compact set $B \subset A \times A$ which contains no diagonal points, there holds $\inf_B w(x, y) > 0$;

4) There is a neighborhood G of the diagonal relative to $A \times A$ such that w is bounded from above on any set $G \setminus (U_{a_1} \cup \dots \cup U_{a_n})$, where U_{a_i} is a neighborhood of the point (a_i, a_i), $i = 1, \dots, n$.

Theorem. *Let $A \subset \mathbf{R}^{d'}$ be a d-rectifiable set and w satisfy conditions 1)–4). Then,*

$$\lim_{N\to\infty} \delta_N^w(A) N^{1/d} = C_d \left(\int_A w(x,x)^d \, d\mathcal{H}_d(x) \right)^{1/d},$$

where constant C_d is the same as in (2).

If $\mathcal{H}_d(A) > 0$, then the density of the limit distribution of optimal configurations is proportional to the function $\rho(x) = w(x, x)^d$, $x \in A$.

Locally-supported wavelets obeying boundary conditions. **Willi Freeden** (TU Kaiserslautern, Germany) IC/MT3718/054

This talk deals with the problem of constructing locally supported wavelets on (regular) regions of the (unit) sphere, thereby obeying certain boundary conditions. As an important application in geosciences, the determination of the Earth's sea surface topography from discrete data of the (geostrophic) oceanic flow is discussed on a local (oceanic) area including boundary effects on, e.g., coastlines.

IC/MP53/015: Mathematical aspects of materials science.

Organiser: Antonio DeSimone (SISSA, Trieste, Italy)
Co-organiser: Stefan Müller (Max-Planck-Institut Leipzig, Germany)

In recent years, materials science has provided fertile grounds for the development of new tools in the calculus of variations, partial differential equations, and applied analysis. These new developments have, in turn, contributed to the advancement of our current understanding of complex material behavior.

Examples range from homogenization theory for the computation of effective macroscopic properties, to y-convergence for the derivation of reduced models, to weak convergence methods for bridging over length and time scales.

The minsymposium will review some of the recent key achievements in this area, examine the current trends, and explore some new promising directions.

Orientable and non-orientable director fields for liquid crystals. **John Ball** (University of Oxford, UK) IC/MT4143/015

Uniaxial nematic liquid crystals are often modelled using the Oseen–Frank theory, in which the mean orientation of the rod-like molecules is modelled through a unit vector field n. This theory has the apparent drawback that it does not respect the head-to-tail symmetry in which n should be equivalent to $-n$; that is, instead of n taking values in the unit sphere S^2, it should take values in the sphere with opposite points identified, i.e. in the real projective plane $\mathbf{R}P^2$. The de Gennes theory respects this symmetry by working with the tensor $Q = s(n \otimes n - \frac{1}{3}\mathbf{1})$. In the case of a non-zero constant scalar order parameter s the de Gennes theory is equivalent to that of Oseen-Frank when the director field is orientable.

We report on a general study of when director fields can be oriented, described in terms of the topology of the domain filled by the liquid crystal, the boundary data, and the Sobolev space to which Q belongs (which in turn prevents or allows certain defects).

This is joint work with Arghir Zarnescu.

Fluid flow within a fluid membrane. **Marino Arroyo** (Universitat Politècnica de Catalunya, Spain), Antonio DeSimone (SISSA, Trieste, Italy) IC/MT3706/015

We study the mechanics of fluid membranes with a particular emphasis on the inner flowŰthe motion of the lipids within the membrane surface. For this purpose, we obtain the equations of motion of a two-dimensional viscous fluid flowing on a curved surface that evolves in time. These equations are derived from the balance laws of continuum mechanics, and a geometric form of these equations is obtained. The partial differential equations that govern the time evolution of a fluid membrane driven by curvature elasticity or line tension are obtained. We apply these equations to the formation of a protruding bud in a fluid membrane, as a model problem for physiological processes on the cell wall. The 2D flow is induced by the change in shape of the surface domain in which the flow takes place. We study the kinetics of the budding process driven by line tension or interfacial energy, assuming that the neck of the bud corresponds to an interface between phases. The rate of the process is set by a balance between viscous dissipation within the fluid membrane and interfacial energy release rate.

Surfactants in foam stability: a phase-field model. **Irene Fonseca** (Carnegie Mellon University, USA) IC/MT1225/015

The role of surfactants in stabilizing the formation of bubbles in foams is studied using a phase-field model The analysis is centered on a van der Walls-Cahn-Hilliard-type energy with an added term accounting for the interplay between the presence of a surfactant density and the creation of interfaces. In particular, it is concluded that the surfactant segregates to the interfaces, and that the prescription of the distribution of surfactant will dictate the locus of interfaces, what is in agreement with experimentation.

Screening induced fluctuations and collisions in Ostwald ripening. **Barbara Niethammer** (Humboldt-Universität zu Berlin, Germany) IC/MT1209/015

The long-time behavior of classical mean field models for domain coarsening displays a sensitive dependence on the initial data. Higher order effects, such as screening induced fluctuations in the particle number densities or collision of domains, are possible mechanism to drive the coarsening system toward a unique self-similar state. In this talk I give an overview of the derivation of corresponding models and the analysis of their long-time behavior. (This is joint work with Juan Velazquez)

IC/MP53/015: Mathematical aspects of materials science. #2

Organiser: Antonio DeSimone (SISSA, Trieste, Italy)
Co-organiser: Stefan Müller (Max-Planck-Institut Leipzig, Germany)

(For abstract, see session #1 above.)

Texture and microstructure: a new paradigm. **David Kinderlehrer** (Carnegie Mellon University, USA), Eva Eggeling (Carnegie Mellon University, USA), Maria Emelianenko (Carnegie Mellon University, USA), Shlomo Ta'asan (Carnegie Mellon University, USA) IC/MT1503/015

Nearly all technologically useful materials are polycrystalline, consisting of small crystallites, called grains, separated by interfaces, the grain boundaries. The energetics and arrangement of this network, its texture, are important factors in material behavior, and constitute the basic problem of microstructure. Experimentall, the inverse relationships between grain boundary populations and energy have been observed for many years. We introduce the grain boundary character distribution (GBCD), a new statistic, and offer compelling evidence for its strong dependence on grain boundary energy. In addition we demonstrate that there are natural laws for texture and the GBCD using large network simulations

Energy scaling and domain branching in shape-memory alloys and type-I superconductors. **Sergio Conti** (Universität Duisburg-Essen, Germany) IC/MT3432/015

Many problems in material sciences are characterized by the spontaneous formation of fine-scale structures, whose topology changes depending on the control parameters. The different patterns can be understood using nonconvex functionals with a singular perturbation, which physically represents surface energy terms. Focusing on two specific examples (shape-memory alloys and fl<ux penetration in type-I superconductors), I shall show how a combination of interpolation inequalities and explicit constructions permits to determine the scaling of the minimal energy with respect to the relevant material parameters, and therefore to predict a phase diagram for the observed microstructure. This talk is partially based on joint work with R. Choksi, B. Kohn, F. Otto, and S. Serfaty.

A damped wave-type limit for Landau–Lifshitz–Gilbert equation. **Antonio Capella Kort** (Universität Bonn, Germany), Felix Otto (Universität Bonn, Germany), Christof Melcher (Humboldt-Universität zu Berlin, Germany) IC/MT2661/015

We discuss the Landau–Lifshitz–Gilbert dynamics of magnetic domain walls driven by small applied fields. In certain regimes and geometric configurations, where one of the magnetization's components is heavily penalized, the interplay between energetic and dynamic forces becomes singular. If the Gilbert damping is sufficiently small, an effective damped wave type dynamics of the nonheavily penalized magnetization's components is observed.

In particular we study the effective dynamics of Néel walls in magnetic thin films. We prove in this case, existence of traveling wave and periodic solutions for small, constant and periodic forcing. We also deduce an asymptotic dynamic law for the wall's center q, of the form

$$M\,\ddot{q} + \frac{1}{\beta}\,\dot{q} = H(t)$$

where, M and β are the effective wall mass and mobility, and H is the applied field. This result suggest that, in this regime the domain wall can be considered as a puere topological object, that behaves as a particle of finite mass. We also give explicit expressions for the wall mass and mobility in terms of the static Néel wall profile and various physical constants.

Oscillatory aspects of Landau–Lifshitz–Gilbert dynamics. **Christof Melcher** (Humboldt-Universität zu Berlin, Germany) IC/MT1386/015

Landau-Lifshitz-Gilbert dynamics is the fundamental evolution law in ferromagnetims. It describes a damped precession of the magnetization vector about the effective field steming from the underlying interaction energy. In the simplest cases the equation can be considered as a hybrid heat and Schrödinger flow for harmonic maps into the sphere. In this talk we discuss analytical features of this equation that lead to typical dynamic phenomena such as oscillatory motion of micromagnetic singulaities or the existence of non-coherent precessional states in the presence of a spin torque.

IC/MP624/005: Approximation and point distribution on the sphere.

Organiser: Ian Sloan (University of New South Wales, Australia)
Co-organiser: Douglas Hardin (Vanderbilt University, USA)

The 2-dimensional sphere is an important setting for applications in geophysics, quantum physics, particle scattering and other fields, yet it presents many mathematical challenges. Many difficulties arise from the absence (except in the special cases associated with the platonic solids) of regular partitions or regular distributions of points on the sphere. Yet progress is being made. This minsymposium will present current research on approximation by polynomials and radial basis fuctions and related methods for partial differential equations on the sphere, together with properties of minimum energy point distributions, and other problems of discretization.

Asymptotics for discrete weighted minimum energy problems on the sphere. **Douglas Hardin** (Vanderbilt University, USA) IC/MT3525/055

Given a closed d-rectifiable set A embedded in Euclidean space (for example, $A = S^d$), we investigate minimal weighted Riesz energy points on A; that is, N points constrained to A and interacting via the weighted power law potential $V = w(x,y)\,|x-y|^{-s}$, where $s>0$ is a fixed parameter and w is an admissible weight. (In the unweighted case ($w \equiv 1$) such points for N fixed tend to the solution of the best-packing problem on A as the parameter $s \to \infty$.) Our main results concern the asymptotic behavior as $N \to \infty$ of the minimal energies as well as the corresponding equilibrium configurations. Given a distribution $\rho(x)$ with respect to d-dimensional Hausdorff measure on A, our results provide a method for generating N-point configurations on A that are "well-separated" and have asymptotic distribution $\rho(x)$ as $N \to \infty$? This is joint work with E. B. Saff and S. V. Borodachov.

Constructive approximations of spherical functions . **Mahadevan Ganesh** (Colorado School of Mines, USA) IC/MT1375/005

Approximation of functions on the sphere arises in almost all applications modeling data collected on the surface of the earth and for reconstruction of various processes in spherical coordinates. Interpolation operators on the circle and periodic domains (based on a class of basis functions and data values) are essential for many high performance simulations. These operators are represented by analytical summation formulas that can be computed very efficiently using the fast Fourier transform. We construct a similar class of interpolation and quasi-interpolation operators on the sphere using a new class of basis functions and demonstrate the power of such operators with several benchmark numerical experiments. This is a joint work with H.N. Mhaskar.

Extremal spherical designs. **Robert Womersley** (University of New South Wales, Australia) IC/MT3128/055

A spherical n-design is a set of m points on the unit-sphere S^2 such that the corresponding equal weight cubature rule is exact for all spherical polynomials of degree at most n. Traditionally the interest has been in finding the points that give the largest value of n for a given m, or equivalently in looking for the smallest number of points m for a given n. Theoretically the best known results valid for all $n \geq 0$ have $m = O(n^3)$, in contrast to the known lower bounds $m \geq n^2/4 + O(n)$, which are not achievable except in a few special cases.

However there is very strong numerical evidence that $m = (n+1)^2$, the dimension of the space of all spherical polynomials of degree at most n, is more that adequate. Moreover this number of points leaves some freedom, which can be used to choose points with another desirable characteristic. One such characteristic is to maximize the determinant of the basis matrix, as is done for D-optimal designs in statistics. The extremal points of Womersley and Sloan, with their (numerically) positive cubature weights, provide excellent starting points for finding extremal spherical designs. Spherical designs are also an example of quasi-Monte Carlo (QMC) points for the sphere.

This talk looks at characterisation of extremal spherical designs with $m = (n+1)^2$ points as constrained global optimization problems. Lobatto like versions, with the additional condition of points at the north and south poles, are also considered. Some of the nice properties of these point sets, which make them suitable for both numerical integration and polynomial interpolation over the sphere, are presented.

Constructive approximation on the sphere. **Ian Sloan** (University of New South Wales, Australia) IC/MT1372/005

As building blocks for approximation on the sphere both radial basis functions (RBF's) and polynomials have their advantages: RBF's are good for scattered data, can be concentrated in regions where the variation is rapid, and can have compact support; while polynomials are good for slowly varying global phenomena. Here, in joint work with Alvise Sommariva, we discuss a constructive hybrid approximation, one that seeks to combine the virtues of both RBF's and polynomials.

05: Applied Analysis, Contributed Talks

IC/CTS4591/05: **Miscellaneous, incl. waves.**

Organiser: Paula Cerejeiras (Universidade de Aveiro, Portugal)

Finite reflection groups and spherical Radon transform. **Paula Cerejeiras** (Universidade de Aveiro, Portugal) IC/CT3576/015

Texture analysis deals with the experimental determination and interpretation of the statistical distribution of orientations of crystals within a specimen of poly-crystalline materials (the orientation of each individual crystal assumed to be unique). The localization can be preformed via the inversion of a spherical Radon transform - a ill-posed problem.

In this talk we study the problem of localization and inversion of the spherical Radon transform under the action of conformal transformations φ_a linked to the special symmetries of the crystal as described by the finite reflection group.

Study of the convergence of a non-iterative splitting scheme. **Elodie Tillier** (Institut Français du Pétrole, France) IC/CT2319/051

The modelisation of the CO_2 geological storage gives a reactive multiphase flow problem. We use to solve it a non iterative splitting method which consist in decoupling the multiphase flow model and the reactive transport model. The error introduced by the splitting is corrected by a penalization term. The objective of this paper is to study the validity of this method. We simplify the full problem in order to be able to make a theoretical study. To do that, we consider just one species which can be present in aqueous and in gaseous phase, and a mineral. We are interested by the equilibrium between the species in gaseous phase and in aqueous phase, and by the kinetic reaction with the mineral. It gives a simplified two phase diffusion-reaction problem. We first write the continuous problem for the splitting method. Then we propose a finite volume scheme. We show that this scheme converges to the weak solution of the initial continuous problem. First, we show that the approximate solution obtain with the splitting scheme converges to the weak solution of the splitting continuous problem, then, by passing to the limit, we show that it also converges to the weak solution of the initial continuous problem. Work done in collaboration with Robert Eymard and Laurent Trenty.

Scattering of flexural gravity waves by abrupt change in water depth. **Trilochan Sahoo** (IIT, Kharagpur, India), Debabrata Karmakar (IIT, Kharagpur, India) IC/CT31/101

In the recent decades, there is a large interest in analyzing wave interaction with large floating flexible structures which has wide application in both ocean engineering and cold region science and technology. In the construction of very large floating structures such as floating airports, the structures are considered flexible in nature. The floating ice sheets that cover a vast area of the ocean surface in the cold regions are also modeled as flexible structures and are used for various human activities. The surface gravity waves originated in the open sea interact with the floating flexible structures and penetrates into the region covered by the flexible structures to generate flexural gravity waves. Chen et al. (2006) reviewed the hydroelasticity theories for global response of marine structures. On the other hand, the various aspects of wave ice interaction problems are investigated by various researchers (see Porter and Porter (2004), Manam et al. (2006) and the literature cited there in) in the recent literature.

In the present paper, the scattering of flexural gravity waves due to an abrupt change in ocean depth is analyzed in case of finite depth in the linearized theory of water waves. In the present paper, Timoshenko–Mindlin equation for the plate equation is used to include shear and inertia effect in the plate equation. The generalized expansion formulae along with the corresponding orthogonal mode-coupling relations are used to obtain the velocity potential for the boundary value problem associated with the physical problem which is also derived based on the direct application of GreenŠs integral theorem. Using GreenŠs identity the relation between reflection and transmission coefficients is obtained which is used for checking the accuracy of the numerical computations.

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Existence of best approximant in a nonconvex domain. **Hemant Kumar Nashine** (Chhattisgarh Swami Vivekanand Univeristy, India) IC/CT2691/015

Theory of approximation is one of the important fields of applied mathematics. The concept of best approximation given by Chebyshev is one of the useful technique among several approximation methods. In 1854, Chebeshev developed the notion of a best approximation of continuous functions by polynomials and established a criterion for polynomial for best approximation in the metric space. Leter its application to the various fields of mathematics, has attracted the analysts and now independent theory of best approximation is taking shape convering various approachs.

The aim of the present note is to establish an existence result on best approximation for the nonexpansive mappings (not necessarily linear), which are noncommuting in the domain of q-normed space following the line of Meinardus.

Iterative methods for solving fractional differential equations. **Varsha Gejji** (University of Pune, India) IC/CT4220/015

Fractional differential equations have gained considerable importance due to their varied applications in visco-elasticity, electro-analytical chemistry, electrical circuits, fractional multipoles, neuron modelling and related areas in physics, chemistry and biology. Numerous problems in physics, chemistry and engineering are modelled mathematically by fractional differential equations. In the present work we study iterative methods to solve fractional differential equations. Especially

the method proposed by Adomian has proven rather successful in dealing with both linear as well as non-linear problems as it provides analytical approximate solutions of nonlinear equations without linearization, perturbation or discretization. We apply Adomian decomposition method for solving fractional differential equations in a variety of cases and provide illustrative examples.

Some recent advances in vector quasi-equilibrium problems. **Abdul Khaliq** (BGSB University Rajouri, India) IC/CT1534/005

Quasi-equilibria constitute an extension of Nash equilibria, which are of fundamental importance in the theory of non-cooperative games. The problems in this area have involved variety of mathematical methodologies. In this paper we survey recent results concerning the existence of a solution to the vector quasi-equilibrium problems. After a brief construction of the main results, direct applications are focused on the existence of solutions to vector equalibrium problems, vector quasi-variational inequality problems and vector optimization problems.

Key words and phrases: Equilibrium problems, quasi-variational inequalities, KKM-Fan theorems, fixed point theorems, upper semicontinuity

2000 Mathematics Subject Classification: 90C29,49J40, 49J35,47J20

IC/CTS4589/05: Asymptotics.

Organiser: Diego Dominici (SUNY New Paltz, USA)

Coarsening dynamics of polymer droplets for a lubrication model with large slippage. **Georgy Kitavtsev** (Humboldt-Universität zu Berlin, Germany), Barbara Wagner (Weierstraß-Institut Berlin, Germany), Lutz Recke (Humboldt-Universität zu Berlin, Germany) IC/CT3938/052

In this talk we analyze the final stages of the dewetting process of nanoscopic thin polymer films on hydrophobized substrates using a lubrication model that captures the large slippage at the liquid-substrate interface. The final stages of this process is characterized by the slow-time coarsening dynamics of the remaining droplets. For this situation we derive a reduced system of equations from the lubrication model, using singular perturbation analysis. Such reduced models allow for an efficient numerical simulation of the coarsening process. The reduced model extends results by Glasner and Witelski [PRE (67):016302,2003] who investigated a no-slip lubrication model. Apart from collapse and collision, we identify here some new coarsening dynamics.

Asymptotic frictional contact models for piezoelectric plates. **Isabel Figueiredo** (Universidade de Coimbra, Portugal), Georg Stadler (University of Texas at Austin, USA) IC/CT2743/052

Piezoelectric materials convert mechanical energy into electric energy and vice-versa. Currently they are widely used as sensors and actuators in engineering applications, as for example aerospace, aeronautic, automotive, industrial, biomedical, underwater communications, medical imaging and control. In this talk we study new asymptotic models for thin plates with piezoelectric patches and layers that are subject to frictional contact with an obstacle. In the asymptotic process, the thickness of a three-dimensional partial differential equation model for a plate is driven to zero and the convergence of the unknowns is studied. This leads to a two-dimensional model in which mechanical displacement and electric potential are partly decoupled. Based on this two-dimensional model we present numerical examples illustrating actuator and sensor capabilities of smart devices with piezoelectric materials in the presence of obstacles.

On relative perturbation theory for block operator matrices. **Luka Grubišić** (RWTH Aachen, Germany) IC/CT3001/052

We use weakly-formulated operator equations to study perturbation problems for 2×2 operator block matrices. We allow (integro) differential operators, defined by quadratic forms, as coefficients in these weak operator equations and block operator matrices. An analysis of the "weakly formulated" Sylvester equation yields new scaling robust bounds for the rotation of spectral subspaces of a nonnegative self-adjoint operator in a Hilbert space. Our bound extends the known results of Davis and Kahan. As an example we give constructive estimates for the convergence rates of eigenvalues and eigenfunctions of the Arch model eigenvalue problem as the diameter of the thin elastic (rod like) body tends to zero. Furthermore, this prototype problem is identified as representative for the whole class of non-inhibited stiff perturbation families. This class of perturbations is characterized by a kind of inf-sup condition. Another problem which we study is bounding a perturbation of the square root of a positive self-adjoint operator. The obtained estimate is also of the relative type and we use a Sylvester like equation to solve this problem (cf. Grubišić, L.; Veselić, K. *On weakly formulated Sylvester equations and applications*, Integral Equations and Operator Theory, to appear, Preprint: http://arxiv.org/abs/math.SP/0507532). This is a joint work with K. Veselić, Hagen, Germany and J. Tambača, Zagreb, Croatia.

Geometrical optics approach to Markov-modulated fluid models. **Diego Dominici** (SUNY New Paltz, USA) IC/CT740/052

We analyze asymptotically a differential-difference equation, that arises in a Markov-modulated fluid model. In the steady state limit, the joint probability distribution of the buffer content and the number of active sources satisfies a system of $N+1$ ODEs, that can also be viewed as a differential-difference equation analogous to a backward/forward parabolic PDE. We use singular perturbation methods to analyze the problem for $N \to \infty$, with appropriate scalings of the two state variables. In particular, the ray method and asymptotic matching are used.

Modulation equations for finite-amplitude nonlinear waves in an incompressible fluid. **Warren Smith** (University of Birmingham, UK) IC/CT1117/052

A formal perturbation scheme is developed to determine original modulation equations for laminar finite-amplitude nonlinear waves in an incompressible fluid. The modulation equations comprise conservation of waves, averaged conditions for conservation of mass, momentum, and kinetic energy and the averaged projection of the Navier-Stokes equations onto the vorticity vector. The last of these modulation equations, which is related to vortex stretching, only appears in three-dimensional problems. The technique of Reynolds averaging is also employed to obtain equations for the mean velocity and pressure. The Reynolds-averaged Navier-Stokes equations correspond to the modulation equations for conservation of mass and momentum. However, the Reynolds stress transport equations are shown to be inconsistent with the other necessary modulation equations.

Derivation of the micropolar shell model. **Josip Tambača** (University of Zagreb, Croatia), Ibrahim Aganović (University of Zagreb, Croatia), Zvonimir Tutek (University of Zagreb, Croatia) IC/CT2010/052

In this work we mathematically derive a two-dimensional model of a shell-like body starting from the three-dimensional linearized micropolar elasticity.

The micropolar elasticity is a theory of solids which in contrast to the classical elasticity uses two kinematical vector fields, displacement and microrotation of the material point and two dynamical vector fields, force and couple. The material points are allowed to rotate without stretch.

The derivation of the 2-D model is based on the asymptotic expansion method with respect to the small parameter. In the present setting the small parameter is the thickness of the shell-like body; it is assumed that the thickness is much greater than the grain size. The behavior of the solution of the 3-D problem is analyzed with respect to the small parameter. The essential role in this analysis is played by the scaling of coefficients, unknowns and loads in the problem. Here the method is used without any *a priori* assumption on the scaling of the unknowns. Instead we use the set of rules, called Ansatz, inspired by the derivation of the classical plate model by Miara.

It turns out that *no scaling* is necessary in contrast to the case of classical elasticity. The form of the leading order displacement and microrotation and their correctors is derived in a classical way. Further we show that the leading term, displacement and microrotation, is the unique solution of certain 2-D problem, called the micropolar shell model. This model can be written in the form which is well defined for shells with $W^{1,\infty}$ middle surface.

We justify the model by showing that the family of solutions of the 3-D micropolar elasticity problem converge to the solution of the obtained 2-D model as the thickness of the shell tends to zero.

IC/CTS4590/05: Wavelets.

Organiser: Bin Han (University of Alberta, Canada)

lossless and near-lossless wavelet-based compression chemes. **Paco Arandiga** (Universitat de València, Spain) IC/CT3048/054

Being able to control the quality of the decoded data instead of the compression rate is suitable for applications where quality control is of utmost importance, yet we would like to be as economical as possible with respect to storage and speed of computation. In this paper we present a compression algorithm based on Harten's interpolatory framework for multiresolution that guarantees a specific estimate of the error between the original and the decoded image measured in the max-norm.

The aim of this talk is to show some of the advantages of this family of transformations when used as lossless and near-lossless image compression technique.

Riesz wavelets in Sobolev spaces. **Bin Han** (University of Alberta, Canada) IC/CT3555/054

Riesz wavelets are of interest in image processing and numerical algorithms for solving partial differential equations numerically. In this talk, we shall present a complete characterization of Riesz wavelets in a Sobolev space $H^s(R)$ for any real number s. Examples of Riesz wavelets derived from B-splines in Sobolev spaces, including the well-known hierarchical basis in the finite element method, will be given to illustrate the results. Interesting connections of Riesz wavelets to tight wavelet frames and refinable functions of exponential decay in wavelet analysis will be also addressed.

About the mathematical foundation of the Hilbert–Huang transform. **Uwe Kähler** (Universidade de Aveiro, Portugal) IC/CT3574/054

In recent years, a new tool has emerged in signal processing, the so-called Huang–Hilbert transform. In difference to classic Fourier and wavelet based methods, the Hilbert spectrum is considered instead of the Fourier spectrum, which makes the method more sensible to non-linear data but also to noise. The heart of Huang's idea is to overcome the problem of constants in the Hilbert transform by a deomposition which is called empirical mode decomposition (EMD). In this talk we will look into the mathematical foundation of the Huang-Hilbert transform and show how methods of Clifford analysis can be used to extend this transform to higher dimensions.

A numerical solution for fractional differential equations. **Hossein Parsian** (Islamic Azad University of Saveh, Iran) IC/CT390/054

In this talk, we present a numerical solution for solving fractional differential equation of order $alpha$ ($n-1 < \alpha < n$ and n is real integer). This method is based on expansion over wavelets. Wavelets constitute a family of function that constructed from dilation and translation of a single function. The mother function of Legendre wavelet is Legendre function. Legendre wavelets are defined over the interval $[0,1]$. In recent years, Legendre wavelets are used for solving differential equations, Integral equations and variational problems. In this research work, we present an operational matrix for fractional derivative. The operational matrix develops the Legendre wavelets formalism to fractional calculus. We formulate this problem in terms of left Riemann-Liouville fractional derivative. Several examples demonstrate the validity of this operational matrix.

Recovery algorithms for vector-valued data with joint sparsity constraints. **Holger Rauhut** (Universität Wien, Austria), Massimo Fornasier (University of Princeton, USA) IC/CT2021/054

Vector valued data appearing in applications often possess sparse expansions with respect to a preassigned frame for each vector component individually. Additionally, different components may also exhibit common sparsity patterns. Recently, there were introduced sparsity measures that take into account such joint sparsity patterns, promoting coupling of non-vanishing components. These measures are typically constructed as weighted ℓ_1 norms of componentwise ℓ_q norms of frame coefficients. We show how to compute solutions of linear inverse problems with such joint sparsity regularization constraints by thresholded Landweber algorithms. Further we discuss the adaptive choice of suitable weights appearing in the definition of the sparsity measures. The weights are interpreted as indicators of the sparsity pattern and are iteratively up-dated after each new application of the thresholded Landweber algorithm. The resulting two-step algorithm is interpreted as a convergent double-minimization scheme for a suitable target functional. Numerical experiments in color image restoration and distributed compressed sensing are presented.

Edge detection. **Zoraida Martínez** (Universidad Simón Bolívar, Venezuela), Carenne Ludeña (IVIC, Venezuela) IC/CT2811/054

In this work we introduce an algorithm for the automatic detection of curves in images based on curvelets (Candès and Donoho) and model selection techniques. Our main interest is detecting curves in noisy environments corrupted by nuissance line segments. Our algorithm is then applied to the automatic selection of events in seismic traces, where the determination of these events is of great importance for characterization of boreholes.

In the first part of our work we consider the method of Energy Functions with Gabor Filters. A close look at the method evidences the importance of directional information.

Motivated by the excellent results obtained with this methodology, in the second part of the work, new methods for curve detection with directional characteristics are explored, such as curvelets and their implementation by contourlets (Vetterli and Do), accompanied with model selection techniques, to obtain an optimal representation of the edges.

Several simulation results show the potential of the proposed algorithm.

IC/CTS4644/05: Wave propagation, scattering, asymptotics.

Organiser: George Makrakis (IACM/FORTH, Greece)

Linear and nonlinear problems of active noise shielding. **Sergei Utyuzhnikov** (University of Manchester, UK), Ali Turan (University of Manchester, UK) IC/CT4274/050

The problem of active shielding of some domain from the effect of the field generated in another domain is considered. The active shielding is implemented via the placement of additional sources in such a way that the total contribution of all sources leads to the desirable effect. Mathematically, the problem is reduced to seeking certain source terms satisfying some *a priori* described requirements and belongs to the class of inverse source problems. From the application standpoint, this problem is closely related to the active shielding of noise, active vibration control and active scattering.

The solution of the problem of active shielding in the differential and finite-difference formulations is obtained under some general conditions. In contrast to many other approaches, it does not require either the knowledge of the particular Green's function or any other information on source distribution and the surrounding medium. It is also important that along with undesirable field to be shielded, a desirable field can be admitted in the analysis. The solution of the problem requires only knowledge of the total field on the perimeter of the shielded domain. The active shielding sources are obtained for both the linear and nonlinear implementations of the problem. In the case of a system governed by first-order equations, the active shielding source term is represented in the form of a single layer. Particular examples of the Helmholtz equation, acoustics equations, Maxwell equations and Euler equations are considered.

Work done in collaboration with V.S. Ryaben'kii.

Transmission operators for description and modeling of 3D scattered acoustic wavefields in layered heterogeneous media. **Milana Ayzenberg** (Norges Teknisk-Naturvitenskapelige Universitet, Norway), Arkady Aizenberg (IPGG, SB RAS, Russian Federation), Jan Pajchel (Norsk Hydro, Norway) IC/CT2395/050

We consider acoustic transmission problem in 3-D layered heterogeneous media with smooth curved interfaces. We rewrite standard statement of the problem by representing the continuity conditions for pressures and normal accelerations at the interfaces in the form of an equivalent linear system of transmission transforms. The transforms are represented by action of the transmission (reflection or refraction) convolution-type operators on the pressures and normal accelerations. Kernels of the operators are the spatial Fourier transforms of the classical reflection or refraction plane-wave coefficients. The representation is based on the fact that in a small vicinity of the interface the pressure and normal acceleration wavefields can be described by the sum of two spectral integrals generalizing the Weyl integrals. Using the Green theorem we may represent the scattered wavefield in each layer by the two surface singular integrals of Kirchhoff type. The boundary values of the integrals satisfy a modified system of the boundary integral equations. The operator of this system contains the classical surface integral propagators and transmission operators. Applying the Neumann method to the system, we obtain the boundary values as a branching sequence of multiple reflections and refractions. For modeling purposes we use a high-frequency approximation of the propagators in the form of the tip wave superposition method. For the transmission operators we use a dominant-frequency approximation in the form of effective coefficients. The effective coefficients generalize the plane-wave coefficients conventionally used in the acoustic and seismic modeling to the case of finite dominant frequency, non-plane interface and arbitrary wavefront of the incident wavefield. Application of the effective coefficients leads to amplitude and phase correction and generation of new wavefields with different kinematics, in particular the head waves. We provide results of numerical modeling of scattered wavefields.

Numerical solution of scattering problems using pseudo-differential impedance operators. **David Calvo** (Naval Research Laboratory, USA) IC/CT2034/050

Direct numerical solution of scattering problems based on integral equation or finite-element formulations are computationally costly at high frequencies. A numerical solution method is presented using high-accuracy pseudo-differential impedance operators (PIO) implemented using rational approximations. An example of a PIO is the so-called on-surface radiation condition (OSRC) method. The method can be viewed as applying a parabolic equation directly on the surface of a scatterer to provide an approximate Dirichlet-to-Neumann map for the scattered field. In contrast to past OSRCs, the use of rational approximations provides accuracy for wide scattering angles which is needed near grazing angles of incidence. Generalization to impedance operators for penetrable scatterers is presented along with applications to scattering from wavy interfaces such as the ocean bottom. Finally, the use of OSRCs as a key ingredient to iteratively solving integral equations for scattering problems is discussed (Antoine & Darbas 2005). [Work sponsored by ONR]

Reconstruction of complex obstacles from scattering data. **Mourad Sini** (RICAM Linz, Austria) IC/CT446/050

The inverse scattering for an obstacle with mixed boundary condition can be considered as a prototype for radar detection of complex obstacles with coated and non-coated parts of the boundary. We construct some indicator functions for this inverse problem using the far-field pattern directly. Based on the careful singularity analysis, these indicator functions enable us to reconstruct the shape of the obstacle and distinguish the coated and the non-coated part of the boundary. Moreover, an explicit representation formula for the surface impedance in the coated part of the boundary is also given. Our recon-

struction scheme reveals that the coated part of the obstacle is less visible than the non-coated one, which corresponds to the physical fact that the coated boundary absorbs some part of the scattered wave. Numerics are presented for the reconstruction formulas, which show that both the boundary shape and the surface impedance in the coated part of boundary can be reconstructed accurately.

This work is done in collaboration with J.J. Liu and G. Nakamura.

Asymptotic expansion of the solution of the Wigner equation near caustics. **George Makrakis** (IACM/FORTH, Greece), Evangelia Kaligiannaki (University of Crete, Greece) IC/CT4224/052

The Wigner transform is employed to reformulate the Cauchy problem for the Schrödinger equation with polynomial potentials and oscillatory initial data in configuration space, as a quantum Liouville (Wigner) equation in phase space. We explain that solutions of the Wigner equation retaining the small parameter can capture the correct Wigner function near and on the caustics, and they can therefore provide the correct energy densities at such singularities. Departing from an eigenfunction series expansion of the Wigner function, we construct asymptotic expansions of the solutions of the Wigner equation for anharmonic potentials using as a datum the Wigner function of the harmonic oscillator. Our analysis gives useful insight concerning the behaviour of the Wigner function on the caustics, and the generation of cusp caustics form the focal points of the harmonic oscillator due to anharmonicity.

Matched asymptotic expansions for the computation of the field scattered by a patch antenna. **Abdelkader Makhlouf** (INSA Toulouse, France) IC/CT3580/052

In this talk we are interested in the computation of the electromagnetic field scattered by a patch antenna (a thin coating partially covered by a perfect conductor). The classical methods (finite differences or finite elements method) require a local refinement of the mesh near the thin coating which leads to expansive computations. Moreover, the technique of equivalent boundary condition (see [1] for example) can not be directly applied due to the presence of singularities near the end of the perfect conductor.We would like to apply the technique of Matched Asymptotic Expansions[3,4] and the technique of singularity computation [2,5] to obtain an asymptotic expansion of the solution.

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05: Applied Analysis, Posters

IC/PP1863/015: Existence of almost-periodic solutions of a delay-differential equation.

Presenter: Abbas Syed (IIT Kanpur, India)

This Poster is to address theoretical issues for functional differential equations, particularly delay-differential equations. Delay-differential equations are very important class of nonlinear differential equations. They arise in many problems, such as population dynamics, biological phenomena from physiology, neural networks and drug release when modeled mathematically. In this poster I also describe some of my recent research results on delay-differential equations.

IC/PP4732/050: Pseudo-differential operator theory in seismic imaging.

Presenter: Chad Hogan (University of Calgary, Canada)
Co-author: Gary Margrave (University of Calgary, Canada)
Co-author: Michael Lamoureux (University of Calgary, Canada)

Many current industrial seismic imaging algorithms rely on wavefield extrapolation, which may be accomplished using a one-way Helmholtz equation. A scalar Helmholtz equation describing wave propagation of a single frequency (ω) wave in two dimensions x, z through a scalar velocity field $v(x,z)$ is used

$$(\partial_z^2 + \partial_x^2 + \omega^2/v(x,z)^2)\phi(x,z) = 0.$$

This equation may be formally factored into two one-way wave equations, e.g. $(i\partial_z + \mathbf{B})\phi^+(x,z) = 0$. $\mathbf{B}$ is a pseudodifferential operator with symbol defined by its square such that the symbol of $\mathbf{B}$, $\Omega_{\mathbf{B}}$, when composed with itself recovers the symbol for the full Helmholtz equation. i.e. $\Omega_{\mathbf{B}}\#\Omega_{\mathbf{B}} = (\omega^2/v(x,z)^2 - \xi^2)$, where ξ is the Fourier conjugate to x.

Solutions for this operator $\mathbf{B}$ may then be used in a phase space path integral formulation to derive a computable algorithm for wavefield extrapolation (i.e. one-way marching). One asymptotic solution for the symbol $\Omega_{\mathbf{B}}$ is

$$\Omega_{\mathbf{B}}(x,z) \sim \sqrt{\omega^2/v(x,z)^2 - \xi^2}.$$

If this symbol is used, the resulting algorithm is

$$\phi^+(x, z+\Delta z, \omega) = \int_R e^{i\Delta z\sqrt{\omega^2/v(x,z)^2-\xi^2}}\hat{\phi}^+(\xi,\omega,z)e^{ix\xi}d\xi.$$

Our research is focussed in two major directions. First, we are interested in numerical improvements in this algorithm in terms of accurately evaluating this integral. Second, we are working to incorporate better asymptotic representations of the symbol $\Omega_{\mathbf{B}}$ for both the range-independent and range-dependent cases.

IC/PP409/052: Spectrum of discrete Sturm–Liouville operators via orthonormal polynomials.

Presenter: Rabah Khaldi (Annaba University, Algeria)

We study the properties of Sturm–Liouville operators using the orthonormal polynomials with respect to a measure on the segment $[-1,1]$ perturbed by an infinite sequence of point masses. Note that the properties of a discrete Sturm–Liouville operators are transformed in a defined way to the continuous Sturm–Liouville operator that is of fundamental importance in mathematics and physics. The spectrum of discrete Sturm–Liouville operators in a particular case have been already studied in [2].

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IC/PP937/052: The Bogolubov generating functional method in statistical physics and collective variables transform within the grand canonical ensemble.

Presenter: Anatoliy Prykarpatsky (WMS AGH/IAPMM, Poland)
Co-author: Nikolay Bogolubov (jr.) (MI Russian Academy of Science)

We show that the N.N. Bogolubov generating functional method [1] is a very effective tool for studying distribution functions of both equilibrium and non equilibrium states of classical many-particle dynamical systems. Let a large system of one-atomic and spinless) bose-particles with a fixed density in a volume be specified by a quantum-mechanical Hamiltonian operator, consisting of the kinetic energey operator and of a two-particle potential energy operator, allowing a partition into a short range potential of the Lennard–Johns type and a long range potential of the Coulomb type. Making use of the second quantization representation, the Hamiltonian operator can be re-written as the operator acting in a suitable Fock space with the standard scalar product, being constructed of the standard creation and annihilation operators. Introduce the Bogolubov generating functional:

$$\mathcal{L}(f) := (\Omega, \exp[i\rho(f)]\Omega) \tag{1}$$

for any *test* Schwartz function $f \in S(\mathbb{R}^3;\mathbb{R})$, where $\rho(f) := \int_{\mathbb{R}^3} \mathrm{d}^3x\, f(x)\,\rho(x)$, then for n-particle distribution function one can get the expression:

$$F_n(x_1,x_2,...,x_n) =: \frac{1}{i}\frac{\delta}{\delta f(x_1)}\frac{1}{i}\frac{\delta}{\delta f(x_2)}...\frac{1}{i}\frac{\delta}{\delta f(x_n)} : \mathcal{L}(f)|_{f=0}\,. \tag{2}$$

The following main propositions are proved.

Proposition *The functional (1) satisfies [1,2] the following functional Bogolubov type equation:*

$$[\nabla_x - i\nabla_x f(x)]\frac{1}{i}\frac{\delta\mathcal{L}(f)}{\delta f(x)} = -\beta\int_{\mathbb{R}^3}\mathrm{d}^3y\nabla_x V(x-y) : \frac{1}{i}\frac{\delta}{\delta f(x)}\frac{1}{i}\frac{\delta}{\delta f(y)} : \mathcal{L}(f)\,,$$

with the expression

$$\mathcal{L}(f) = Z(f)/Z(0), \quad Z(f) := \exp[-\beta V(\delta)]\mathcal{L}_0(f)\,,$$
$$\mathcal{L}_0(f) = \exp(z\int_{\mathbb{R}^3}\mathrm{d}^3x\{\exp[if(x)]-1\})$$

being its exact functional-analytic solution.

Proposition *Let the Bogolubov-type generating functional $\mathcal{L}(f)$, $f \in S(\mathbb{R}^3;\mathbb{R})$, represented analytically as a series of graph-generated functionals, satisfy the following conditions: 1. continuity with respect to the natural topology; 2. positivity; 3. symmetry and normalization conditions; 4. translational-invariance; 5. cluster condition or, equivalently, the Bogolubov correlation decay; 6. the equilibrium density condition.*

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06: Optimization, Minisymposia

IC/MP341/010: Advances in interior point methods.

Organiser: Florian Potra (National Institute of Standards and Technology, USA)

The advent of interior-point methods has revolutionized the field of mathematical programming. Over the past two decades algorithms and software for linear programming based on interior-point methods have become quite sophisticated, while extensions to more general classes of problems, such as convex quadratic programming, semidefinite programming, and nonconvex and nonlinear problems, have reached varying levels of maturity. The minisymposium speakers will present new advances in this field, focussing on the relation between different formulations of the cone programming problem and the relation between computational complexity and the geometrical properties of the central path, The impact of the theoretical results on the design of more efficient algorithms will be emphasized.

First-order primal–dual algorithms for cone programming. **Renato Monteiro** (Georgia Institute of Technology, USA) IC/MT1610/010

In this talk, we consider the general cone programming problem, and propose primal-dual convex (smooth and/or nonsmooth) minimization reformulations for it. We then survey first-order methods suitable for solving these reformulations, namely, Nesterov's optimal method, Nesterov's smooth approximation scheme, and Nemirovski's prox-method, and propose a new variant of Nesterov's optimal method which has outperformed the latter one on our computational experiments. We also derive iteration-complexity bounds for these first-order methods for solving the proposed primal-dual reformulations. The performance of the variants obtained in this way is then compared using a set of randomnly generated linear programming (LP) and semidefinite programming (SDP) instances. We also compare the approach based on the variant of Nesterov's optimal method with the low-rank method proposed by Burer and Monteiro.

Interior point methods for linear complementarity problems. **Florian Potra** (National Institute of Standards and Technology, USA) IC/MT2666/010

We present a class of interior point methods for solving general linear complementarity problems over symmetric and nonsymmetric cones that admit self-concordant logarithmically homogenous barriers. The methods use adaptive long steps to produce iterates in a wide neighborhood of the central path. We present results on the computational complexity of the algorithms from this class, and give sufficient conditions under which the duality gap converges superlinearly to zero. We also give sufficient conditions for the convergence of the iterates produced by the interior point methods under consideration.

Geometric structure of the central trajectories and complexity of interior-point. **Takashi Tsuchiya** (Inst. of Statistical Mechanics, Tokyo, Japan) IC/MT2668/010

Sonnevend, Stoer and Zhao introduced a curvature integral of the central trajectory for LP which provides an approximation to the iteration-complexity of interior-point algorithms. Monteiro and Tsuchiya studied the curvature in relation with the Vavasis–Ye's layered-step interior-point algorithm, and established an interesting property that the total curvature of the central trajectory is bounded by $O(n^{3.5}L_A)$, where n is the number of nonnegative variables and L_A is the imput bit length of A. In this talk, we discuss further implications and extensions of this result.

IC/MP309/010: Applied topological methods.

Organiser: Victor Zvyagin (Voronezh State University, Russian Federation)

The minisymposium is intended to present a large variety of applications of contemporary topological methods to some problems, such as: control theory, hydrodinamics, variational inequalities. In this perspective we will present latest applications of the topological degree theory and the coincidence index to some optimization and controllability problems for control systems governed by differential inclusions in finite and infinite-dimensional spaces. The other applications are connected with the finding of optimal feedback control in problems arising from models of non-Newtonean visco-elastic fluids. Also we will describe topological methods which are applicable for solving the problems described by variational inequalities and their applications in optimization and mathematical economics.

Investigation of boundary value problems for certain models of non-Newtonian hydrodynamics. **Victor Zvyagin** (Voronezh State University, Russian Federation) IC/MT546/010

The report devoted to the description of contemporary investigations in the field of new boundary and initial-boundary value problems for stationary and evolution equations of non-Newtonean hydrodynamics. In particular, we present the investigation of the following problems:

1. The solvability of boundary value stationary problem with slip for the model of electro-rheological fluid;
2. The investigation of initial-boundary value problem in the model of motion of viscoelastic fluid with JeffreyŠs constitutive relation;
3. The description of trajectory and global attractors for the Jeffreys model;
4. The investigation of the initial-boundary value problem for the Voight model in the case of varying domain;
5. The study of some optimal feedback control problems in the Voight model.

All results are obtained by the following approximate-topological method. At first we give the operator treatment of the considered problem in the form of the operator equation in some functional space which is appropriate for this problem. For this equation we suggest a family of auxiliary operator equations defined in a functional space which has (as a rule) better topological properties. Further, the application of some versions of the topological degree theory in Banach spaces and *a priori* estimates allow us to obtain the solvability of these auxiliary equations. At last, the passage to the limit (in the sense of distributions theory) in the sequence of solutions of auxiliary equations, based on *a priori* estimates of these solutions in the initial functional space, leads to the solution of the principal operator equation and, hence, to the solution of the initial problem.

Relative topological degree and variational inequalities. **Pietro Zecca** (Università di Firenze, Italy) IC/MT1686/010

We give a definition of relative topological degree for multimaps which are composition of approximable multimaps and continuous maps. Then, we apply this notion to prove an existence result for variational inqualities of Stampacchia's type of the form:

(S) Let V be a normed space, $K \subset V$ a nonempty, closed convex set, $h \in V$ a given element, $T : V \multimap V$ a multimap.

Find $x \in V$, $y \in T(x)$ such that

$$\langle v - x, y \rangle \geq \langle v - x, h \rangle \quad \forall v \in K.$$

Some applications to optimization problems are considered.

Attractors of boundary-value problems for motion equations of a few viscoelastic media models. **Dmitry Vorotnikov** (Voronezh State University, Russian Federation) IC/MT968/010

We shall describe sufficient conditions for existence of minimal uniform trajectory attractors and uniform global attractors of evolution equations which do not have uniqueness of Cauchy's problem. Unlike the earlier results (e.g. [1]), here it is not assumed that the symbol space of an equation is a compact metric space and that the family of trajectory spaces corresponding to this symbol space is translation-coordinated or closed in any sense. We shall also discuss the case of autonomous equations, which is simpler than the general case. In this situation any invariance of the trajectory space of an equation is not required. Then we shall show some results on properties and structure of the attractors. Application of this theory allows us to construct attractors for weak solutions of the boundary value problems for the motion equations of an incompressible viscoelastic medium with the Jeffreys constitutive law [2] and more complicated constitutive laws.

A significant part of the talk will be based on works [3],[4]. The research was partially supported by grants 04-01-00081 (RFBR), VZ-010-0 (Ministry of Education and Science of Russia and CRDF) and MK-3650.2005.1 (Grant of President of Russian Federation).

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[3] Vorotnikov, D., Zvyagin V., Trajectory and global attractors..., *J. Math. Fluid Mech.* (to appear, published on the journal web-page).

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Multi-valued variational inequalities and applications. **Irene Benedetti** (Università di Modena e Reggio Emilia, Italy) IC/MT2189/010

This talk deals with applications of multivalued variational inequalities of Stampacchia's type to a boundary value problem for a PDE of the form

$$\begin{cases} -\Delta u + f \in \Psi(u), & x \in \Omega \\ \dfrac{du}{dn} \geq 0, & x \in \partial\Omega \end{cases}$$

where $\Omega \subset \mathbb{R}^n$ is a bounded domain with a regular boundary $\partial\Omega$, $u \in W^{1,2}(\Omega, \mathbb{R})$, $f : \mathbb{R}^n \to \mathbb{R}$, $\Psi : W^{1,2}(\Omega, \mathbb{R}) \multimap W^{1,2}(\Omega, \mathbb{R})$ are given function and multifunction.

IC/MP309/010: Applied topological methods. #2

Organiser: Victor Zvyagin (Voronezh State University, Russian Federation)

(For abstract, see session #1 above.)

Existence and uniqueness of a weak solution for the model of Foight. **Mikhail Turbin** (Voronezh State University, Russian Federation) IC/MT990/010

In connection with the presence of a large number of physics applications many papers recently attend to the study of liquid motion in domain with time-dependent boundary. In the majority of works in the given direction the resolvability of Navier–Stokes equations in similar domains is investigated. Namely in works [1,2,3] various statements of initial boundary value problems have been offered and existence of strong and weak solutions and some regularity problems have been investigated. However Nuton model of liquid motion does not describe the motion of liquids possessing relaxation or retardation properties for example of various gels and emulsions.

We study the initial-boundary value problem for Foight mathematical model in domains with time-dependent boundary is investigated. This model describes the motion of a liquid to which needs time to begin a motion under the action of suddenly applied force.

The main result is the existence and uniqueness theorem of the weak solution for this initial boundary value problem. For the proof we consider an approximation problem and show its resolvability using the topological degree theory and *a priori* estimates of solutions. Then we show that the solution of this approximating problem converges to the solution of our starting problem.

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Mathematical modelling of slipping of nonlinear-viscous fluids. **Mikhail Kuzmin** (Voronezh State University, Russian Federation) IC/MT3998/010

The mathematical model of non-stationary (and stationary) movement of nonlinear-viscous fluids under conditions of slip on the boundary is considered. Various types of conditions of slip are considered. Theorems of existence of initial-boundary (and boundary) problems describing movement of nonlinear-viscous fluids under condition of slip on the boundary are proved. For this purpose the approximating-topological method is used.

Differential inclusions on Riemannian manifolds. **Andrei Obukhovskii** (Voronezh State University, Russian Federation) IC/MT3999/010

I consider second-order differential inclusions on a Riemannian manifold with Carathéodory and lower semicontinuous right hand sides. Several existence theorem for solutions of two-point boundary value problem are proved that are interapted as controllability of special mechanical systems with control on nonlinear configuration spaces. As an application a statement of controllability under extreme values of controlling force is obtained.

[1] 1]1 Yuri E. Gliklikh, Andrei V. Obukhovskii; On Two-Point Boundary Value problem for Second-Order Differential Inclusions On Riemannian Manifolds. Abstract and Applied Analysis 10 (2003), pp.591–600.

IC/MP339/015: Industrial organization and game theory.

Organiser: Alberto Pinto (Universidade do Porto, Portugal)

The Stackelberg (1934) model is one of the most widely used models in industrial organization for analysing firms' behaviour in a competitive environment. It studies the strategic situation where firms sequentially choose their output levels in a market. The question we ask is: Do first movers really have strategic advantage in practice? The belief of first-mover advantage was widely held among entrepreneurs and venture capitalists, but is now questioned by numerous practitioners. Several research papers focus their attention in giving answers to such question. Liu (2005) studied the effects of the market demand uncertainty to explain the advantages and disadvantages of being the leading firm.

The Cournot competition with R&D investment programs consists of two subgames in one period of time. The first subgame is an R&D investment program where both firms have initial production costs and choose, simultaneously, the R&D investment strategies to obtain new production costs and at what moment of the period is achieved the reduction. We present new deterministic and stochastic dynamics on the production costs of Cournot competitions using Nash equilibrium of R&D investment strategies with and without uncertainty of the firms. At every period of time, the firms invest in R&D projects to reduce their production costs. The R&D strategies of the firms give rise to deterministic and stochastic dynamics on the production costs characterizing the duopoly competition along the periods of the time. We studied the effect of the dynamics in the profits and persistence of the firms in the market.

Scientific objectives: To extend Liu's results by focus not only on the effects of the market demand uncertainty, but also on product differentiation, to explain the advantages and disadvantages of being the leading firm. To extend the results on the previous item to other models, including private information, signalization, and international competition with subsidies and tariffs. To prove analytically the empirical results already obtained. To extend the results on the previous item to other models, including private information, signalization, and international competition with subsidies and tariffs.

An approach to different voting rules from cooperative games with alternatives. Discussion case: the Catalonia parliament. **Antonio Magana** (Universitat Politècnica de Catalunya, Spain), Francesc Carreras (Universitat Politècnica de Catalunya, Spain) IC/MT2195/015

Classical cooperative (simple) games cannot cope with certain subtleties of voting rules. The structure of such a game, given by a list of *winning* coalitions, doesnŠt specify the inputs for voters, the feasible outputs and the mechanism that transforms any set of inputs in a well defined output. Roughly speaking, these games merely describe the case where a proposal is faced to a status quo or the case where a proposal has to be chosen among several ones by absolute or qualified majority. Thus, e.g., the abstention possibility or the decision-making by the usual relative majority rule cannot be represented this way. As a consequence, when applied to these games, classical power measures as the Shapley–Shubik index may well fail to reflect accurately the strategic position of the voters. This is an important limitation in the analysis of shareholder corporations, political organisms and voting bodies in general.

Games with alternatives provide a wider framework that allows us to describe voting rules precisely. The natural extension of the Shapley–Shubik index to this class of games, axiomatically founded, becomes an interesting tool for a numerical evaluation of the strength of each voter in any system. These ideas will be illustrated on a real life numerical example, the Catalonia Parliament. By considering different voting rules scheduled by the Parliament By-Laws, modelling them by means of suitable games with alternatives, and applying the extended Shapley–Shubik index, remarkable differences between the voters will be discovered that depend on the voting procedure considered.

Asymmetric dynamic price competition with uncertainty. **Fernanda Ferreira** (Instituto Politecnico do Porto, Portugal), Flávio Ferreira (Instituto Politecnico do Porto, Portugal), Miguel Ferreira (Universidade do Porto, Portugal), Alberto Pinto (Universidade do Porto, Portugal) IC/MT3561/015

In this paper, we consider a price competition in a duopoly with substitutable goods, linear and asymmetric demand and with unknown costs. One of the firms is a leader: it chooses first the price p_1 for its product; and the other firm is a follower: it chooses the price p_2 for its product after have observed the price p_1. We suppose that each firm has two different technologies, and uses one of them following a certain probability distribution. The use of either one or the other technology affects the unitary production cost. We show that there is exactly one perfect Bayesian equilibrium for this game. We analyse the variations of the expected market prices and the expected profits over the probability distributions' parameters, and also over the demand parameters. We show that for production costs with the same average, the expected profit of the leading firm increases with the variance of its production costs, and the expected profit of the follower increases with the variance of both production costs.

Two main utility-sharing methods in joint business: a discussion. **Francesc Carreras** (Universitat Politècnica de Catalunya, Spain), Rafel Amer (Universitat Politècnica de Catalunya, Spain), Antonio Magana (Universitat Politècnica de Catalunya, Spain) IC/MT1029/015

The proportional rule has a long tradition in collective problems where utility (costs, profits, savings) is to be shared among the agents. While its apparent simplicity may be a reason for applying it in pure bargaining affairs, where only the whole and the individual utilities exist, it seems much more questionable in case of general cooperative problems, where all marginal contributions should matter.

The axiomatic foundation proposed by Shapley, when introducing the value notion for cooperative games, allows us to discuss positive and negative aspects of the proportional rule and compare it with the Shapley value.

Shapley stated the general problem of finding a value; i.e., a rule for allocating to each cooperative game a payoff vector for its players. He imposed four reasonable conditions a value

should satisfy: efficiency, null player property, symmetry, and additivity. Moreover, he proved an existence and uniqueness theorem: there is one and only one rule that fulfils these requirements.

In this framework, the proportional rule can be checked and compared with the Shapley value. The proportional rule:

(a) applies only on a restricted domain of games;
(b) ignores almost all marginal contributions of the players, so that valuable agents in a cooperative affair may well be not rewarded;
(c) exhibits a hardly justified double discriminatory level;
(d) coincides with the Shapley value on additive or symmetric games;
(e) satisfies efficiency, the null player property and symmetry in its restricted domain;
(f) fails to satisfy additivity, which is not merely a standard mathematical property but one of great interest for practitioners since, from the lack of additivity, serious inconsistencies derive when applying the rule to related cost and saving problems, purchasing pools making accumulated orders, or sharing costs in simultaneous supplies.

IC/MP339/015: Industrial organization and game theory. #2

Organiser: Alberto Pinto (Universidade do Porto, Portugal)

(For abstract, see session #1 above.)

Emergence of long-run behaviours in a game-theoretic setting with host and guest populations: residents and tourists. **Elvio Accinelli** (Universidad Autonoma de San Luis Potosi, Mexico) IC/MT4096/015

In this paper we model tourism development in the framework of multi-population dynamics and analyze the time pattern of its impact as the evolution of the interaction between two populations feeding over the same space-resource. Each population might be structured in two (or more) clubs with variable membership, a club being a group of population members sharing social and economic interests as to the management of the relevant resource. Thus, each club has in principle a different set of strategies as to protection and valorization of broadly defined environmental resources at the tourist destination. Such resources share some of the characteristics of the so called commons. To represent such peculiar situation, we use Evolutionary Game Theory, in particular as is applied to the theory of evolution of interacting structured populations. In one such game, one strategy will be characterized as conservative and its alternative as depredative. Interaction between different strategies and the corresponding playing clubs gives rise to a rich dynamics, as some joint outcomes are inherently unstable, as is known, others being evolutionary stable. Such situation will be modeled by a version of the well known replicator dynamics, to emphasize its evolutionary nature.

Strategic trade policy and signalling costs with differentiated goods. **Flávio Ferreira** (Instituto Politecnico do Porto, Portugal), Fernanda Ferreira (Instituto Politecnico do Porto, Portugal), Alberto Pinto (Universidade do Porto, Portugal) IC/MT853/015

We consider two Cournot firms, one located in the home country and the other in the foreign country, producing differentiated goods for consumption in a third country or market. At the beginning of period 1, the home government commits to a subsidy for the home firm. At this stage neither the home government nor the foreign firm knows the cost of the home firm, though it is common knowledge that it has either low (c_L) or high (c_H) costs with Prob$(c = c_L) = \phi$. Marginal cost of the foreign firm is common knowledge. At the end of the first period, both firms make their output decisions simultaneously, to maximise profits. After observing the output levels of the home firm, the uninformed agents update their beliefs about the costs of the home firm. Let $\phi(q_1)$ be the common updated probability assessment, where q1 is the first-period output of the home firm. At the beginning of the second period, based on the updated beliefs, $\phi(q_1)$, the home government sets its policy instrument level to maximise welfare. Given the subsidy level chosen by the home government and given the updated beliefs of the foreign firm, the two firms choose period 2 outputs to maximise profit.

Donald Wright (1998) analysed the case of homogeneous goods, and showed that, in such case, the optimal subsidy is lower when the home firm signals costs compared to the case when the firm does not. In our work, we show that if the goods are differentiated, the optimal subsidy can be higher when the home firm signals costs compared to the case when the firm does not.

Firms signaling earnings. **Nuno Azevedo** (Ponte de Lima, Portugal), Alberto Pinto (Universidade do Porto, Portugal) IC/MT860/043

The signaling models are under criticism as the empirical literature found weak evidences supporting a central prediction: the positive relationship between changes in dividends and changes in earnings. In the absense of single-crossing property, signaling is possible, and changes in dividens and changes in earnings can be positively or negatively related.

Optimal investments in repeated Cournot competition. **Alberto Pinto** (Universidade do Porto, Portugal), Bruno Oliveira (Universidade do Porto, Portugal), Fernanda Ferreira (Instituto Politecnico do Porto, Portugal), Flávio Ferreira (Instituto Politecnico do Porto, Portugal), Miguel Ferreira (Universidade do Porto, Portugal) IC/MT859/015

We present deterministic dynamics on the production costs of Cournot competitions, based on R&D investment strategies of the firms. In this paper, we focus our attention in the drastic long term economic effects resulting from starting with different initial production costs. We find three distinct economic regions, in the space of all possible initial production costs for both firms, consisting of a no survival, weak survival and recovery behavior. The survival boundary for firm F_1 is the boundary between the no survival and weak survival regions for firm F_1, and is characterized by the stable manifold of the "last" no survival equilibrium. The recovery boundary for firm F_1 is the boundary between the weak survival and survival regions for firm F_1, and is determined by the stable manifold os the "last" weak equilibrium. This characterization of the economic boundaries through the stable manifolds of equilibrium points shows a nice interplay between dynamics and economics. The recovery region for firm F_1 is a set of initial production costs for both firms in which the firm F_1 is with initial production costs worse than the firm F_2, but after some periods of time the firm F_2 is able to diminish the gap between the two firms and both firms approach production costs favourable to both firms. The weak survival region of firm F_1 corresponds to initial production costs where the gap between the initial production costs of the firms is greater than in the survival region. Along the time the gap increases and the production costs of the firms approach a region of production costs which are unfavourable to firm F_1 and favourable to firm F_2.

IC/MP262/015: Applied mathematics in Latin America: part 2.

Organiser: Domingo Tarzia (CONICET - Univ. Austral, Rosario - ARGENTINA)
Co-organiser: Julio Claeyssen (Universidade Federal do Rio Grande do Sul, Brazil)

The goal of this minisimposium (Part 2) is to give an overview of the state of the art in diferent subjects related to partial differential equations, optimization and optimal control that are under current development in several regions of Latin America.

Convergence of boundary-optimal controls in mixed elliptic problems. **Claudia Gariboldi** (Universidad Nacional de Río Cuarto, Argentina), Domingo Tarzia (CONICET - Univ. Austral, Rosario - ARGENTINA) IC/MT599/015

We consider the problems P and P_α respectively with mixed boundary conditions (for each parameter $\alpha > 0$):

$$-\Delta u = g \; in \; \Omega \quad u|_{\Gamma_1} = b \quad -\frac{\partial u}{\partial n}|_{\Gamma_2} = q$$

and

$$-\Delta u = g \; in \; \Omega \quad -\frac{\partial u}{\partial n}|_{\Gamma_1} = \alpha(u-b) \quad -\frac{\partial u}{\partial n}|_{\Gamma_2} = q$$

where $g \in L^2(\Omega)$, $q \in L^2(\Gamma_2)$ and $b \in H^{\frac{1}{2}}(\Gamma_1)$.
We consider q as a boundary control variable for suitable cost functionals J and J_α which depend on the solution of problems P and P_α respectively for each positive $q \in L^2(\Gamma_2)$. We formulate boundary optimal control problems. We prove the existence and uniqueness of the boundary optimal controls q_{op} and q_{op_α} (for each parameter $\alpha > 0$) and we give the optimality conditions as complementary conditions in terms of the optimal controls and the optimal adjoint states $p_{q_{op}}$ and $p_{q_{op_\alpha}\alpha}$ of the systems, respectively. We also prove that the optimal control q_{op_α} and its corresponding system state $u_{q_{op_\alpha}\alpha}$ and adjoint state $p_{q_{op_\alpha}\alpha}$ are strongly convergent to $q_{op}, u_{q_{op}}$ and $p_{q_{op}}$ in $L^2(\Gamma_2), H^1(\Omega)$ and $H^1(\Omega)$ respectively when $\alpha \to \infty$.

The HIV-1 dynamics as an optimization process. **Federico Biafore** (Universidad Nacional de San Martín, Argentina), DAttellis Carlos (Universidad Favaloro, Argentina) IC/MT3733/036

The dynamics of the HIV-1 infection can be represented by means the use of predator-prey models that represent the interaction of the virus and the host immune system. The values of the parameters of this models are obtained using regression techniques from experimental data and/or adjusted by the researcher with the purpose of reproducing the infection dynamics observed in the clinical practice. The aim of this work is to try to reproduce the dynamics of the infection expressing the infection rate parameter of the employed model as a variable that evolves according to an optimization approach. The Maximum Pontryagin Principle is applied. The preliminary results suggest the possibility to explain some aspects of the HIV-1 dynamics as an optimization process involving a cost function.

An improved scheme for accelerating the convergence of the simulated annealing algorithm applied to real-world problems. **Adriana Verdiell** (Universidad Nacional del Sur, Argentina), María Maciel (Universidad Nacional del Sur, Argentina), Marta Vidal (Universidad Nacional del Sur, Argentina) IC/MT758/015

When formulated in mathematical terms, the problem of zoning a protected natural area subject to both box and spatial constraints results in a large combinatorial optimization problem belonging to the NP-hard class. These facts suggest the need to apply a heuristic approach. In this contribution a new proposal to decrease the control parameter, known as temperature, in the simulated annealing algorithm is presented. The strategy is based on that proposed by Lundy and Mees, and developed in order to decrease the running time of the algorithm applied to large scale problems. When applied to solving small-size simulated problems, results were indistinguishable from those obtained via an exact, enumerative method.

A coarse-scale zoning of Talampaya National Park (Argentina) rendered maps remarkably similar to those produced by subject area experts using a non-quantitative consensus-seeking approach. Results are encouraging and show particular potential for the periodical update of zoning of protected natural areas. Such a capability is crucial for application in developing countries where both human and financial resources are usually scarce but still critical for updating zoning and management plans.

Numerical approximation of a variational problem. **Lisandro Parente** (Universidad Austral de Rosario, Argentina), Laura Aragone (Universidad Austral de Rosario, Argentina), Pablo Lotito (UNICEN de Buenos Aires, Argentina), Gabriela Reyero (Universidad Nacional de Rosario, Argentina) IC/MT585/015

We consider a variational analysis problem which generalizes the problem of optimal Lipschitz extension. More precisely we consider the minimization of a functional given by $J(u) = \operatorname{ess\,sup}_{x\in\Omega} f(x,u,Du)$ where $u \in W^{1,\infty}_g = \{v \in W^{1,\infty} : v = g \text{ on } \partial\Omega\}$ and $\Omega \subset \mathbb{R}^n$ is bounded. In the particular case that $f(x,u,Du) = \|Du\|$ the problem becomes the search for the Lipschitzian extension of g with minimum Lipschitz constant.

This work deals with the numerical approximation of the solution. The optimality conditions of this problem are given by the Aronson-Euler equation. One approach could be to look for a viscosity solution of these equations. Instead, given the quasiconvexity of the data functions, we can solve it as a finite dimension optimization problem obtained through the discretization of the original one.

The obtained optimization problem can be nonlinear depending on the function f. In order to solve it we penalize the restrictions and consider the system of nonlinear equations given by the optimality conditions. We show that the penalized solution converges to the solution of the discretized problem, and we solve the nonlinear equation system by a Newton type method.

We present results on the convergence rate of our numerical method that depends on the regularity of the functional. We show some numerical examples.

IC/MP204/061: Multidisciplinary optimization in simulation-based design.

Organiser: Natalia Alexandrov (NASA Langley Research Center, USA)

Complex engineering design optimization problems, especially problems governed by computational simulations, rarely lend themselves to straightforward formulation and solution by conventional methods of nonlinear programming. Multidisciplinary optimization (MDO) comprises methods from computational optimization, disciplinary and process modeling, and various engineering disciplines that govern different aspects of a system being designed. In this minisymposium, we dis-

cuss the challenging analytical and computational aspects of multidisciplinary simulation-based design problems, as well as techniques for solving some classes of these problems. The techniques include exploiting problem structure, alternative problem formulation, the use of various approximations and multi-physics models to address the cost of expensive simulations (e.g., the solution of differential equations), and the use of computational infrastructures. Applications that serve to illustrate the use of methods include aerospace problems and ship-design problems.

Multilevel methods for PDE-constrained optimization. **Natalia Alexandrov** (NASA Langley Research Center, USA) IC/MT1457/061

We examine an approach to the design of complex systems governed by coupled PDE. The term multilevel refers to the optimization problem formulation, the solution algorithm and the use of several layers of models in representing a particular discipline at various stages of design. We investigate analytical and computational properties of the approach and examine a numerical demonstration.

High-fidelity modeling and parallel architecture in the simulation-based design of a fast multi-hull ship. **Daniele Peri** (INSEAN, Italy), Antonio Pinto (INSEAN, Italy), Giovanni Fasano (INSEAN, Italy), Emilio Campana (INSEAN - Italian Ship Model Basin, Italy) IC/MT362/061

Design activities of marine veichles usually involve many different disciplines, highly interacting each other. In this context, design optimization meets great difficulties due to the requested effort. Fast, multihull ships are the today's trend for displacement marine vehicles. However, if the space between the hulls is small, interference effects arise, generated both by the interaction between the boundary layers of the two hulls and by the two wave systems interaction. This leads to an increase in the total resistance of the ship that has to be minimised. Furthermore, also the effect of the real pitch angle and draught the ship has once at speed must to be accounted for. As a consequence, expensive RANS solvers, with free-sufrace capturing capacities and also able to handle the free-running model, are mandatory, which implies a dramatic increase of the total cost of the optimization cycle: to this aim, a number of different techniques have been developed in the field of Multi-Objective Design Optimization in order to alleviate the computational cost of the whole optimization cycle. In this paper, a real-life optimization problem for the shape optimization of a fast catamaran ship is tackled. Parallel architectures, in conjunction with metamodel techniques are applied. A mixed strategy, with the use of two different derivative-free global optimization algorithms, is presented. Preliminary results demonstrate the great improvements the designer may obtain by controlling the different elements of the interference between the hulls.

Particle-swarm optimization method in the MDO of a sail-boat keel. **Giovanni Fasano** (INSEAN, Italy), Emilio Campana (INSEAN - Italian Ship Model Basin, Italy), Daniele Peri (INSEAN, Italy), Antonio Pinto (INSEAN, Italy) IC/MT375/061

We consider the use of a class of global optimization techniques, for the minimization of a nonconvex function, arising from a ship design real application. The latter problem comes up in a large number of practical ship design and naval engineering contexts, where different disciplines must be often coupled, encompassing hydrodynamic and structural problems. This scenario requires the use of specific multidisciplinary formulations, where the approaches with standard mathematical programming methods could be unsuitable. MultiDisciplinary formulations require indeed the combined use of effective Optimization techniques (MDO), in order to solve highly nonconvex and possibly nondifferentiable problems. We propose in this work the use of an optimization method, for the design of a sailboat keel. The formulation of the latter problem provides a global optimization application, whose solution can be hardly tackled with standard techniques, which require the continuous differentiability of the objective function. We applied a modified Particle Swarm Optimization (PSO) method, which owes its popularity to the reasonable balance it provides between the overall computational cost and the quality of the final solution. Despite some recent variants, the algorithms in the PSO class are mainly heuristics, whose progress may be eventually very slow. The latter drawback can be explained by observing that these techniques completely disregard any condition related to first order information on the objective function. We first give a numerical experience which proves the computational efficiency of our proposal. Then we prove that in a linesearch framework and under mild assumptions, our proposal retains the global convergence to stationary points.

A framework for automatic implementation of MDO architectures. **Joaquim Martins** (University of Toronto, Canada) IC/MT1785/061

A new MDO framework has been developed in Python to provide a platform for comparisons relating the performance of various MDO architectures. The framework eliminates the need for problem reformulation when solving MDO problems in multiple architectures. Once a problem has been described, the implementation in any architecture is automatic. In addition to providing a performance comparison of the more common architectures, the modular design of the framework allows rapid testing of newly developed architectures. Results generated from this study provide a strong foundation for identifying the performance trends of various architectures with a variety of problem classes. It also serves to verify the performance and potential of those tested.

IC/MP3439/061: Optimal control of industrial applications modelled by ODEs and PDEs.

Organiser: Kurt Chudej (Universität Bayreuth, Germany)
Co-organiser: Christof Büskens (Universität Bremen, Germany)

Optimization and optimal control of huge realistic models of industrial applications are challenges for applied mathematiciens. Although the applications come from different fields like container cranes, cars and power plants, the mathematical problems are very similiar. A generalization of theory and algorithms is necessary to cope with the enormes complexities of the models.

Hybrid solution of bilevel optimal-control problems. **Matthias Knauer** (Universität Bremen, Germany), Christof Büskens (Universität Bremen, Germany) IC/MT3454/061

The industrial application of container cranes requires the calculation of time and energy optimal trajectories, so that the crane system comes to be at rest at a predefined location. Additionally, it has to be ensured that the crane system can be brought to rest at a free but admissible location within a given time from any state of the trajectory.
This task can be considered as a bilevel optimal control problem: In this extension to classical optimal control problems, additional constraints are considered which depend on the optimal solutions of secondary optimal control problems.

By evaluating the necessary conditions for the secondary optimal control problems, the bilevel structure can be reduced to a single level.

Advanced optimal feedback control for tracking of real-life applications. **Christof Büskens** (Universität Bremen, Germany), Ramona Stach (Universität Bremen, Germany) IC/MT3451/061

Calculating the open-loop solution of an optimal control problem is just the first step to cope with the practical realization of real life applications. Feedback controllers, like the classical Linear Quadratic Regulator closed-loop controller (LQR), are needed to compensate perturbations appearing in reality. Although these controllers have proved to be a powerful tool in many applications and to be robust enough to countervail most differences between simulation and practice, they are not optimal if disturbances in the system data occur. If these controllers are applied in a real process, the possibility of data disturbances force recomputing the feedback control law in real-time to preserve stability and optimality, at least approximately. For this purpose, a numerical method based on the parametric sensitivity analysis of nonlinear optimization problems is suggested to calculate higher order approximations of the feedback control law in real-time. Using this method, the optimal controller can be adapted within a few nanoseconds on a typical personal computer. The method is illustrated by the adaptive optimal control of the classical inverted pendulum and a crane system.

Model reduction in laser welding. **Verena Petzet** (Universität Bayreuth, Germany), Hans Josef Pesch (Universität Bayreuth, Germany) IC/MT3462/061

Laser welding is a modern joining technique for new metallic materials particularly aluminum alloys. However, there is a high risk of hot cracking. Therefore, the aim is to avoid this undesirable effect caused by several processes during the solidification. For modeling process there are three main aspects which has to be considered: The thermodynamical, the mechanical and the metallurgical effect by which the arising of the opening displacement caused by transverse tensile strains can be described. Because of the high complexity of this physical process a model reduction in the mathematical model has to be done.
After that formulation a method can now be applied to prevent hot cracking. One possibility is to use the so called multi-beam technique. Thereby, additional laser beams are imposed to compensate for the strain induced by the main laser beam. Hereby, it is important to determine the optimal position, size and power of the additional laser beams in order to prevent hot cracking. Mathematically, this leads to a constraint nonlinear optimization problem where amongst other constraints a partial differential equation has to be solved.

Optimal control of a servo drive system with Coulombic friction and state constraints. **Helmut Maurer** (Universität Münster, Germany), Oliver Zirn (Universität Gießen, Germany) IC/MT4174/061

We consider a servo drive system that represents a typical electrodynamic actuator. As such an actuator is very common for loudspeakers, it is called a voice-coil-motor. The basic dynamical model comprises five ODEs for the motor, resp., load mass positions and velocities as well as the coil current. The control function is given by the voltage input. The system involves static Coulombic friction that causes discontinuities in the dynamic equation for the motor mass velocity. We study both time-minimal and energy-minimal controls and show that time-minimal controls are of bang-bang type. We present numerical methods for efficiently computing the switching times of the control input and those times where the motor velocity changes sign. When imposing state constraints on the velocities, the optimal control becomes a rather complex combination of bang-bang and boundary arcs. The computed optimal controls were implemented on a real system and turned out to be in perfect agreement with measured test bench results.

IC/MP331/061: Modelling and design of complex systems.

Organiser: Michel Delfour (Université de Montréal, Canada)

The design of endoprotheses in biomechanics or complex mechanical structures such as tires for cars require careful mathematical and reliable numerical modelling from basic physical or biological principles that preserve the essential features without unduely increasing the size of the model in order to be able to successfully handle the numerical optimization/design stage. Examples will be given from interventional cardiology and the tire manufacturing industry.

Adaptive finite-element method for free-surface problems. **André Fortin** (Université Laval, Canada) IC/MT334/061

An adaptive finite element method for the simulation of various free surface problems will be presented. A level set method is used to compute the position of free surfaces. The mesh is adapted at each time step in order to concentrate the mesh at the interface. This allows to impose interface equilibrium conditions with very good accuracy. Various applications will be presented: drop to drop interaction in fluid flow problems, phase change in cryotherapy, die swell of viscoelastic fluids, etc.

Simulation of aerosols in the airway tract with a 3D Eulerian model. **Yves Bourgault** (Université d'Ottawa, Canada), Marc Thiriet (Université Paris VI, France) IC/MT1980/061

The numerical prediction of the propagation of aerosols in airways is an area of growing interest [1,2]. For instance, predicting the deposition patterns of particles in the mouth-throat or the inner lung pathways is needed for designing inhalers. Indeed recovering experimental deposition patterns, both in vivo and in vitro, happens to be difficult and expensive, and one often has to rely on numerical models of gas-particle flows for predicting such patterns in a cost-effective way. Two approaches are commonly used to model such multiphase flows, namely the Eulerian and Lagrangian approaches, but much of the literature on aerosols in airways rely on the Lagrangian tracking approach [1,2]. A common justification for the use of

the Lagrangian approach is that air flows in airways are internal and pulsatile, and present reverse flow regions, potentially leading to crossing particle trajectories. These arguments have been partly waived by a recent paper [3]. An Eulerian model could provide a competitive approach to compute internal dilute gas-particle flows, even in the presence of recirculations. In [4], we obtained numerical results of gas-particle flows in a 2-D prototype airway using a FEM for an Eulerian model.

In the current paper, we will extend our previous Eulerian model to the aerosol propagation in 3-D patient-based geometries of the airway tract. In [5], CT images of the thorax were processed to generate the geometry of the trachea and the first six bronchus generations. The air flow was then obtained by solving the Navier-Stokes equations for different values of the flow dimensionless parameters. In this paper, numerical results for aerosol propagation in these geometries are obtained by coupling our Eulerian model with the previous flow solutions. The results show that the particle density and deposition patterns are easily obtained at all time steps without any need for particle count or the delicate selection of initial particle positions, as for the Lagrangian tracking approach.

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Time-dependent flow simulation in a carotid bifurcation. **Andre Garon** (École Polytechnique de Montréal, Canada) IC/MT354/061

We present the finite element flow simulation in a carotid bifurcation. This time-dependent simulation will be compare to 3D time-resolved PIV measurement for validation and accuracy evaluation. We will discuss the effect of newtonian versus non-newtonian model on the shear-stress at the bifurcation for different LVAD(left ventriculat assist device) support.

Modelling and design of stents in interventional cardiology. **Michel Delfour** (Université de Montréal, Canada) IC/MT332/061

Stents are used in interventional cardiology to keep a diseased vessel open. New stents are coated with a medicinal agent to prevent early reclosure due to the proliferation of smooth muscle cells. It is recognized that it is the dose of the agent that effectively controls the growth. This paper focusses on the asymptotic behavior of the dose for general families of coated stents under a fixed ratio between the coated area of the stent and the targeted area of the vessel and set therapeutic bounds on the dose. It generalizes the results of Delfour, Garon, and Longo (SIAM J. Appl Math) for stents made of a sequence of thin equally spaced rings to stents with an arbitrary pattern. It gives the equation of the asymptotic dose for a normal tiling of the target region.

IC/MP331/061: Modelling and design of complex systems. #2

Organiser: Michel Delfour (Université de Montréal, Canada)

(For abstract, see session #1 above.)

Fluid–kinetic models for sprays. **Laurent Boudin** (Université Paris VI, France) IC/MT4460/061

Fluid-kinetic models are often used when small particles or droplets evolve in an ambient fluid. That situation happens in medicine (therapeutic aerosols in the airways), but also in the military industry. Some examples within those frameworks will be investigated during the talk.

The standard fluid quantities, like mass density ϱ or velocity u, are solutions of the Euler or Navier-Stokes equations.

The spray of particles is described through a kinetic equation, typically, a fitted Vlasov equation

$$\partial_t f + v \cdot \nabla_x f + \nabla_v \cdot (f\gamma) + \partial_r (f\Phi) = 0,$$

where f denotes the particle probability density function, depending on time t, and on the location x, velocity v and characteristical size r of the particles. The acceleration γ holds information about the action of the fluid on the spray, and Φ describes the evolution of r.

The interaction between the two phases can be taken into account in mainly two ways. The first relevant question would be: can the action of the spray on the be neglected with respect to other phenomena? The second one: is the volume occupied by the spray neglictible with respect to the volume of the fluid?

We shall mainly present three different models which are used in the frameworks we already evoked, and eventually show some numerical results.

On the numerical simulation of the electro-cardiogram. **Miguel Fernández** (INRIA Rocquencourt, France), Muriel Boulakia (Université Pierre et Marie Curie, France), Jean-Frédéric Gerbeau (INRIA Rocquencourt, France), Najib Zemzemi (INRIA Rocquencourt, France) IC/MT4766/061

In this work we address the numerical simulation of electrocardiograms (ECG). We consider the bidomain equations to model the electrical activity of the heart and a Laplace equation for the torso. The ionic activity is modeled with the Mitchell-Schaeffer model. We use adaptive semi-implicit BDF schemes in time, finite elements in space, and a Neumann-Robin domain decomposition algorithm for the heart-torso coupling. The obtained ECGs, although not completely satisfactory, are promising. They allow to discuss various modelling assumptions, for example the relevance of cells heterogeneity, fiber orientation and the coupling conditions with the torso.

From reductionism to integrative modeling of living tissues. **Marc Thiriet** (Université Paris VI, France) IC/MT4768/061

Nowadays, most of the computational simulations related to physio/ pathophysiological problems are carried out in three-dimensional model of the subject anatomy obtained by 3D reconstruction from medical image acquisition. Imaging indeed yields the anatomy of the targeted organ, which more or less strongly varies between human subjects. However, these so-called subject-specific computational works deal with a frosen state of the explored organ. Biological tissues are living, and quickly adapt to environmental stimuli. In blood flows, the endothelium is subjected to both chemical cues from neighboring tissues or flowing blood and physical stresses applied by the blood. the endothelial cell changes its shape and gene expression in order to produce molecules which regulate flowing cell extravasation and aggregation, the vasomotor tone of adjoining smooth muscle cells, the substrate transport, and the composition of the extracellular matrix. Moreover, hypoxia, among other factors, leads to angiogenesis, a process in which endothelial cells are particularly implicated. Integrative model of behaviour of living cells subjected to mechanical loading and chemical signaling from themselves, their local environment, and the body regulation system.

A comparison of error estimators for the anisotropic mesh adaptation in 3D compressible flow simulations. **Yves Bourgault** (Université d'Ottawa, Canada), Frédéric Alauzet (INRIA Rocquencourt, France), Adrien Loseille (INRIA, France), Marco Picasso (École Polytechnique Fédérale de Lausanne, Switzerland) IC/MT1966/027

Anisotropic mesh adaptation has proved to be a powerful strategy to improve the quality and efficiency of finite element methods [1]. These anisotropic mesh adaptation techniques were initially based on a metric derived from a numerical approximation of the Hessian of the solutions with, in the background, the use of *a priori* error estimates [1]. More recently, anisotropic *a posteriori* error estimators were derived and used to drive anisotropic mesh adaptation (see [2] and references therein). Both error estimation techniques turned out to be effective, but as far as we know, comparisons of these two approaches have not yet been done in the literature, especially for complex 3D phenomena.

It is the purpose of the current paper to compare adapted meshes and solutions for 3D external flows around a supersonic aircraft, as obtained with different error estimators. We use, among others, the most recent *a priori* error estimators developed in [3] and the anisotropic *a posteriori* error estimators of [2]. Compressible flows are computed using the vertex-centred finite volume method presented in [4]. Comparison of the estimators are made on the basis of the quality of the solutions and computational requirements. The anisotropic adapted meshes are obtained in a solver/mesher loop with the *mmg3d* mesh adaptation software. That software implements the local mesh modification techniques presented in [1]. The goal of the project is to develop simulation capabilities for complex 3D external flows that run on simple workstations in a limited time and with limited memory.

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IC/MP78/061: PDE-constrained optimization: numerical analysis and scientific computing.

Organiser: Roland Griesse (RICAM Linz, Austria)
Co-organiser: Arnd Rösch (RICAM Linz, Austria)

The optimization and control of processes described by partial differential equations plays a key role in understanding complex physical phenomena, the creation of new industrial products and materials, and the enhancement of production cycles. In addition, PDE-constrained optimization is gaining importance in biology, medicine and finance. The enormous advances in scientific computing as well as computing hardware allow to attack truly large-scale optimization problems today. In particular, the development of preconditioning and domain decomposition strategies, and the parallelization of optimization algorithms permit the solution of problems with up to billions of unknowns. Simultaneously, the numerical analysis of PDE-constrained optimization problems has made substantial progress. This concerns in particular the development of discretization and regularization techniques, error estimates and the convergence analysis of numerical methods. The goal of this minisymposium is to bring together leading experts and junior scientists from both areas, scientific computing and numerical analysis in PDE-constrained optimization. The speakers will give an overview of recent results in error and convergence analysis, computational techniques, and their application to areas such as crystal growth, hyperthermia cancer treatment and large-scale source inversion problems.

Uncertainty estimation for large-scale PDE-constrained inverse problems. **Omar Ghattas** (University of Texas at Austin, USA) IC/MT3545/061

We address the problem of estimating model uncertainty for large-scale inverse problems governed by PDEs. The approach is based on low rank estimates of the reduced Hessian, which exploit the compact character of the data misfit term of many ill-posed inverse problems. This low-dimensional representation of model uncertainty can be used to facilitate uncertainty propagation. Applications are given to data assimilation problems for contaminant tranport.

Numerical analysis and algorithms in control and state-constrained optimization with PDEs. **Michael Hinze** (Universität Hamburg, Germany) IC/MT3553/061

We propose a tailored discrete concept for optimization problems with nonlinear PDEs including control and state constraints. Its key idea consists in conserving as much as possible the structure of the infinite-dimensional KKT (Karush-Kuhn-Tucker) system on the discrete level, and to appropriately mimic the functional analytic relations of the KKT system through suitably chosen Ansätze for the variables involved. We provide numerical analysis, including convergence proofs and adapted numerical algorithms. As a class of model problems we consider optimization with (nonlinear) elliptic and parabolic pdes. This allows to validate and to compare our concepts against existing approaches for the class of elliptic and parabolic control problems.

Inexact Kleinman–Newton solvers for Riccati equations. **Ekkehard Sachs** (Universität Trier, Germany & Virginia Tech, USA) IC/MT3569/061

Many optimal control problems involving PDEs require in practice the computation of feedback laws for an optimal control. This is achieved through the solution of a Riccati equation which can be large scale, since the discretized problems are large scale and require special attention in their numerical solution. The Kleinman-Newton method is a classical way to solve a Riccati equation. We extend this method to an inexact version and allow the subproblems to be solved by an iterative solver like Smith's method. A prototype of this method shows a substantial reduction of the numerical effort.

Hierarchical space mapping in state constrained optimal control. **Arnd Rösch** (RICAM Linz, Austria), Michael Hintermüller (Universität Graz, Austria) IC/MT3612/061

The space mapping approach for the minimization of complex systems is extended to a hierarchical framework which allows to take various, hierarchical model simplifications into account. The general framework is then applied to Moreau-Yosida regularized state constrained optimal control of PDEs, where the model hierarchy is induced by the regularization parameter and the mesh-size of discretization. The resulting method is of multilevel type and uses an inexact trust region technique for globalization. The talks ends by a report on numerical results.

IC/MP78/061: PDE-constrained optimization: numerical analysis and scientific computing. #2

Organiser: Roland Griesse (RICAM Linz, Austria)
Co-organiser: Arnd Rösch (RICAM Linz, Austria)

(For abstract, see session #1 above.)

Interior-point methods for semi-infinite problems with PDE constraints. **Martin Weiser** (Zuse-Institut Berlin, Germany) IC/MT1424/061

The talk will address interior point methods for semi-infinite programs arising from optimal control problems with state constraints and finitely many controls. It will be shown that locally self-concordant integrated barrier functions can be constructed in a neighborhood of a generic optimal solution. An important point is that the barrier function depends on the spatial dimension of the constraints. Finally, numerical examples will be given.

On saturation effects in the Neumann boundary control of elliptic optimal control. **Mariano Mateos** (Universidad de Oviedo, Spain), Arnd Rösch (RICAM Linz, Austria) IC/MT1648/061

A Neumann boundary control problem for a linear-quadratic elliptic optimal control problem in a polygonal domain is investigated. The main goal is to show an optimal approximation order for discretized problems after a postprocessing process. It turns out that two saturation processes occur: The regularity of the boundary data of the adjoint is limited if the largest angle of the polygon is at least $2\pi/3$. Moreover, piecewise linear finite elements cannot guarantee the optimal order, if the largest angle of the polygon is greater than $\pi/2$. We will derive error estimates of order h^σ with $\sigma \in [3/2, 2]$ depending on the lagest angle and properties of the finite elements. Finally, numerical test illustrates the theoretical results.

A regularization method for elliptic boundary-control problems with point-wise state constraints. **Fredi Tröltzsch** (TU Berlin, Germany), Irwin Yousept (TU Berlin, Germany) IC/MT3372/061

A Lavrentiev type regularization technique for solving elliptic boundary control problems with pointwise state constraints is considered. The main concept behind this regularization is to look for controls in the range of the adjoint control-to-state mapping. By the associated transformation, the problem becomes equivalent to a control-constrained one. After investigating the analysis of the method, a semismooth Newton technique based on the optimality conditions is presented. The theoretical results are confirmed by numerical tests. Moreover, they are validated by comparing the regularization technique with standard numerical codes based on the discretize-then-optimize concept.

Optimal control of temperature distribution in seeded sublimation growth processes of semiconductor single crystal. **Irwin Yousept** (TU Berlin, Germany), Christian Meyer (Weierstraß-Institut Berlin, Germany) IC/MT3441/061

The talk concerns the optimization of a class of nonlinear state-constrained control problems with nonlocal radiation interface conditions, which arise from crystal growth processes by the physical vapor transport (PVT) method. Mainly, due to the interface conditions and the presence of state constraints, the analysis of such problems is quite challenging. The main goal of the talk is to discuss the optimality conditions for the problem and based on them some numerical experiments are carried out.

IC/MP452/061: *Max-flow–min-cut* for continuous flows and related problems.

Organiser: Bernd Kawohl (Universität zu Köln, Germany)
Co-organiser: Gilbert Strang (Massachusetts Institute of Technology, USA)

A continuous maximum-flow problem finds the largest t such that $\operatorname{div} v = t\,F(x,y)$ has a solution in a plane domain Ω, satisfying a constraint $\|(v_1, v_2)\| \le c(x,y)$. The dual problem finds a cut ∂S of minimum capacity. At optimality, the minimum cut is filled to capacity by the maximum flow through S.
This model problem (a continuous version of the Ford-Fulkerson *max flow–min cut* theorem for flows on graphs) has recently found applications in medical imaging and in the modelling of landslides. It is connected with the construction of Cheeger sets, which minimize the ratio of perimeter divided by area among all subsets of Ω.

It is the purpose of the minisymposium to present recent results and open problems on *max flow–min cut* theorems and Cheeger sets.

Minimum cuts and maximum area. **Gilbert Strang** (Massachusetts Institute of Technology, USA) IC/MT488/061

The oldest competition for an optimal shape (area-maximizing) was won by the circle. We want to give the thousandth proof!

Then we measure the perimeter in different ways, which changes the problem (and has applications in medical imaging). If we use the line integral of $|dx| + |dy|$, a square would win. Or if the boundary integral of $\max(|dx|, |dy|)$ is given, a diamond has maximum area. When the perimeter = integral of $\|(dx, dy)\|$ around the boundary is given, the area inside is maximized by a ball in the dual norm.

The second part describes the **max flow-min cut theorem** for continuous flows. Usually it is for discrete flows on edges of graphs. The maximum flow out of a region equals the capacity of the minimum cut. This duality connects to the isoperimetric problems that produce minimum cuts. But the flows are hard to find and a prize is unclaimed.

Discrete approximations to continuum optimal flow. **Ross Lippert** (Massachussetts Inst. Tech., USA) IC/MT1615/061

Problems in partial differential equations with inequality constraints can be used to describe a continuum analog to various optimal flow/cut problems. While general concepts from convex optimization (like duality) carry over into continuum problems, the application of ideas and algorithms from linear programming and network flow problems is challenging. The capacity constraints are non-linear (but convex).

In this talk, I will present an investigation of a discretized version of the planar maximum flow problem which preserves the non-linear capacity constraints of the continuum problem. The resulting finite-dimensional problem can be cast as a second-order cone programming problem or a quadratically constrained program. Good numerical results can be obtained using commercial solvers. These results were in good agreement with the continuum theory of a "challenge" problem posed by Strang.

Cheeger's constant, the continuous max flow-min cut theorem and the Makai-Hayman-Osserman inequality. **Daniel Grieser** (Carl von Ossietzky Universität Oldenburg, Germany) IC/MT3484/061

For a domain in Euclidean space, or a Riemannian manifold with boundary, Cheeger's constant gives a lower bound for the first Dirichlet eigenvalue of the domain. The question arises how to find lower bounds for Cheeger's constant. A very simple, but not well-known idea is to use certain 'test vector fields' for this. The continuous version of the max flow min cut theorem then states that a vector field exists for which the estimate obtained in this way is sharp.

We will also show how a modification of this idea gives a new proof of the inequality of Makai (often attributed to Hayman or Osserman), which bounds the first eigenvalue of a plane, simply connected domain from below in terms of the inradius.

Explicit solutions of the equation $-\operatorname{div} z = f$ under side-constraint $\|z\| = 1$. **Zoja Milbers** (Universität zu Köln, Germany) IC/MT1693/061

We consider the variational problem:

$$E(u) := \int_\Omega d|Du| + \int_{\partial\Omega} \left| u^{\partial\Omega} \right| \mathrm{d}x \to \text{Min!}, \quad u \in BV(\Omega),$$

$$G(u) := \int_\Omega |u| \mathrm{d}x = 1\,.$$

The formal Euler-Lagrange equation to this nonsmooth problem would be

$$-\operatorname{Div}\left(\frac{Du}{|Du|}\right) = \lambda \frac{u}{|u|}\,.$$

However, it is known that a suitable multiple of the characteristic function χ_C of the Cheeger set C of Ω is a minimizer of the variational problem and the Euler-Lagrange equation is not well defined for $u = \chi_C$. A suitable substitute for the Euler-Lagrange equation is given by the substitute equation

$$-\operatorname{Div} z(x) = \lambda S(u(x)),$$

where S on the right hand side is any measurable selection of the set-valued sign function $\operatorname{Sgn}(u(x))$, $z \in L^\infty(\Omega, \mathbb{R}^n)$ with $\|z\|_{L^\infty(\Omega,\mathbb{R}^n)} \le 1$, and $\lambda = E(u)$. The purpose of the present work is the investigation of the vector field z associated with the minimizers of the variational problem. In my talk, after recalling the known results, I construct solutions z of the substitute equation for different measurable selections for the square and show that for each measurable selection S one can find infinitely many vector fields z satisfying the substitute equation on Ω.

IC/MP452/061: *Max-flow-min-cut* for continuous flows and related problems. #2

Organiser: Bernd Kawohl (Universität zu Köln, Germany)
Co-organiser: Gilbert Strang (Massachusetts Institute of Technology, USA)

(For abstract, see session #1 above.)

On facet breaking for crystalline mean curvature flow in 3D. **Giovanni Bellettini** (Dipartimento di Matematica, Universita' di Roma To, Italy) IC/MT2278/061

We analyze some examples of facet breaking/bending of a polyhedral set evolving by crystalline mean curvature in three dimensions. This problem is strictly related to understand which facets of the crystal admit a vector field with constant divergence and satisfying suitable convex constraints. Work in collaboration with M. Novaga (Dipartimento di Matematica, Università di Pisa, Largo B. Pontecorvo 5, 56127 Pisa, Italy, E-mail: novaga@dm.unipi.it) and M. Paolini (Dipartimento di Matematica e Fisica, Università Cattolica di Brescia, via Trieste 41, 25121 Brescia, Italy E-mail: paolini@dmf.unicatt.it).

Convex calibrable sets in $\mathbb{R}^N$ and uniqueness of Cheeger sets inside convex bodies. **François Alter** (CMLA - ENS Cachan, France) IC/MT3630/061

The total variation approach to image denoising can be written as the minimization problem

$$\min_{u \in BV(\mathbb{R}^N) \cap L^2(\mathbb{R}^N)} \int_{\mathbb{R}^N} |Du| + \frac{1}{2\lambda} \int_{\mathbb{R}^N} (u - f)^2 \, dx, \qquad (1)$$

where $f \in L^2(\mathbb{R}^N)$ is the image to be denoised and $\lambda > 0$ is a regularization parameter. The search for explicit solutions of (1) leads to a series of interesting geometric problems related to the characterization of calibrable sets in $\mathbb{R}^N$. A convex body in $\mathbb{R}^N$ is calibrable if for any $\lambda > 0$ its denoising is written as a multiple of itself. Calibrable sets immediately give explicit solutions of (1). We provide a geometric characterization of convex $C^{1,1}$ calibrable sets in $\mathbb{R}^N$ in terms of the mean curvature of its boundary, extending Giusti's result in $\mathbb{R}^2$. We also prove the uniqueness of Cheeger sets inside a convex body in $\mathbb{R}^N$. This result permits to solve the capillary problem in

absence of gravity and vertical contact angle inside a convex Cheeger set, having a geometric characterization of those sets in terms of the mean curvature of its boundary.

Discrete and continuous parametric max-flow. **Antonin Chambolle** (École Polytechnique, France) IC/MT2303/061

The parametric max flow algorithm has been introduced by Gallo, Grigoriadis and Tarjan in order to solve quickly successive graph cuts problems with monotone capacities. It relies on a simple comparison principle for cuts in the same graph, with different outgoing capacities (from the source). We will describe in this talk the continuous version of this principle, and show if time permits how it can be applied for studying (both theoretically and numerically) the solutions of Total Variation minimization problems, with convex penalization. The main collaborator on this study is Jérôme Darbon (UCLA).

Cheeger sets and their construction. **Bernd Kawohl** (Universität zu Köln, Germany) IC/MT1389/061

Given a domain Ω, its Cheeger set is defined as the subset D of Ω, which minimizes perimeter over volume among all subsets. This geometric variational problem arises as a limit problem, as $p \to 1$, for eigenfunctions of the p-Laplace operator. In my lecture I will present examples of Cheeger sets and discuss their uniqueness and explicit construction. Part of this work was obtained jointly with Thomas Lachand-Robert.

IC/MP1015/061: Optimal control with PDEs on gas networks.

Organiser: Jens Lang (TU Darmstadt, Germany)
Co-organiser: Alexander Martin (TU Darmstadt, Germany)

This minisymposium is concerned with the solution of optimization and control problems for flow processes in gas networks. Gas flow problems on networks are described by a hierarchy of local dynamics (PDEs or ODEs) on the edges and transmission conditions at the nodes of the network. The overall dynamics is optimized by discrete decision variables and by continuous control variables according to a certain target functional. Global solutions of corresponding optimization and control problems are obtained by a hierarchy of combinatorical and continuous methods. The successful solution of such complex problems requests the combination of mathematical modelling, mixed-integer optimization, discrete and continuous control theory and numerical mathematics. New mathematical challenges as well as actual solution strategies will be discussed.

Multiscale models for simulation and optimization of gas networks. **Michael Herty** (TU Kaiserslautern, Germany), Axel Klar (TU Kaiserslautern, Germany) IC/MT1530/061

We are interested in gas flow in pipe networks. Several models for the dynamics inside the pipe are known which range from partial differential equations to purely algebraic relations. Usually, the dynamics of different pipes is coupled at pipe fittings and we discuss the mathematical and physical reasonable coupling conditions in particular for nodes which model compressors. We are interested in questions of well-posedness and existence of solutions near such nodes with respect to the different known models. We present numerical simulation and optimization results for compressor control based on the introduced model hierarchy.

Gas optimization by mixed integer-programming techniques. **Alexander Martin** (TU Darmstadt, Germany) IC/MT3118/061

We focus on the combinatorics in the gas optimization problem, that is on the questions which of the compressors to switch on or off and which of the valves to open or close in order to cost-efficiently satisfy all customer demands. We model these decisions as a mixed integer program (MIP) by approximating the inherent nonlinearities by piece-wise linear functions. We solve the resulting MIP by primal and dual methods including branch-and-cut and report on computational results for realistic networks.

Adaptive linearized models for optimization of gas networks. **Oliver Kolb** (TU Darmstadt, Germany), Jens Lang (TU Darmstadt, Germany) IC/MT2644/061

We are interested in simulation and optimization of gas networks. Usually, a gas network consists of different components like compressors and valves connected by pipes. The aim is to run the network cost efficiently whereas demands of consumers have to be satisfied. This results in a complex nonlinear mixed integer problem. We address this task with methods provided by discrete optimization. Therefore, the gas dynamics in all pipes must be described by piecewise linear constraints. We introduce an adaptive approach for the linearization process to handle the complexity on the one hand and the aimed accuracy on the other. We present numerical simulation and optimization results based on our model.

Optimal control of networks of gas pipelines. **Siarhei Dymkou** (Universität Erlangen–Nürnberg, Germany), Günter Leugering (Universität Erlangen–Nürnberg, Germany) IC/MT2230/061

We consider the optimization and control of gas-flow in networks of pipelines. The main objective is to maximize the throughput through the pipeline from the providers to the customers by choosing proper valve- and release-configurations as well as compressors in order to maintain the pressure in given bounds. This problem is considered in the context of bilevel optimization. In particular, after a discretation of the governing partial differential equations on the entire network, we obtain a discrete in space and time dynamical network-flow problem which is optimized with respect to compressor-data and valve-activities taking into account bounds on the discrete flow variables. On the second level, we consider, wherever the flow characteristics make it necessary, the continuous model (or a hierarchy of finer discretizations of it) to which, in turn, we apply continuous as well as switching controls.

IC/MP259/061: Multigrid/multilevel approaches to the optimization of systems governed by partial differential equations.

Organiser: Robert Lewis (College of William and Mary, USA)
Co-organiser: Stephen Nash (U.S. National Science Foundation)

This minisymposium examines multigrid/multilevel techniques in the optimization of systems governed by partial differential equations (PDE). The governing PDE introduces structure to the optimization problem hat can make the latter amenable to solution via multigrid/multilevel techniques. The situation is made more interesting by the fact that these types of optimization problems may involve discretized optimization decision variables, in addition to the discretized state variables representing the solution of the PDE. The talks in this minisymposium discuss the analytical and computational aspects of applying multigrid/multilevel techniques in the context of optimization.

One-shot multigrid method for aerodynamic shape optimization. **Subhendu Hazra** (Universität Trier, Germany) IC/MT1850/061

This talk presents a numerical method for aerodynamic shape optimization problems. It is based on simultaneous pseudo-time stepping in which stationary states are obtained by solving the pseudo-stationary system of equations representing the state, costate and design equations. The main advantages of this method are that it blends in nicely with previously existing pseudo-time stepping method for state and costate equations, that it requires no additional globalization in the design space, and that a preconditioner can be used for convergence acceleration which stems from the reduced SQP methods. To accelerate further the convergence of the method, 'optimization based' multigrid strategy is used. In this method, different optimization problems of similar structure are formulated at different discretization levels. Each of these optimization problems is solved using simultaneous pseudo-time stepping method. The coarse grid problems are computationally less expansive and helps in finding the optimal direction of the fine grid problems faster. For design examples of 2D problems, the overall cost of computation can be reduced to less than 2 times the forward simulation runs.

Multilevel algorithms for large-scale interior-point methods in bound constrained optimization. **Eldad Haber** (Emory University, USA) IC/MT4103/061

We develop and compare multilevel algorithms for solving bound constrained nonlinear variational problems via interior point methods. Several equivalent formulations of the linear systems arising at each iteration of the interior point method are compared from the point of view of conditioning and iterative solution. Furthermore, we show how a multilevel continuation strategy can be used to obtain good initial guesses (Şhot startsŤ) for each nonlinear iteration. A minimal surface problem is used to illustrate the various approaches.

Length-scale and spatial locality effects in the optimization of systems governed by differential equations. **Robert Lewis** (College of William and Mary, USA) IC/MT2447/061

We discuss locality and non-locality in frequency and space in the optimization of systems governed by differential equations. These analytical features have their origin in the abstract nature of the reduced Hessians that arise in the nonlinear programs describing such problems. These analytical features, in turn, have consequences for the development of multi-scale / multigrid schemes for the optimization of systems governed by differential equations. We present analytical and numerical results that suggest why, in many cases, we can be hopeful that multi-scale methods will be effective for such optimization problems. We also discuss why, in other situations, an element of domain decomposition is needed.

IC/MP1050/043: Preconditioned iterative methods for PDE constrained optimization.

Organiser: Marcus Sarkis (WPI/USA and IMPA/Brazil)
Co-organiser: Xiao-Chuan Cai (University of Colorado at Boulder, USA)

Among optimization problems with constraints, those constrained by nonlinear partial differential equations are very challenging, both mathematically and computationally. Examples of such problems are inverse, optimal design and optimal control problems. In inverse problems some parameters of the governing equations of the system behavior are not known and must be estimated by analysis of experimental system output data. Optimal design problems usually refer to problems where the variable is the shape of a domain and one has to find the best shape that minimizes or maximizes an objective function. In optimal control problems one usually searches for the best feasible control variables, such as boundary values or external forces that minimize or maximize a certain system behavior, such as turbulence. The focus of this minisymposium will be on the recent development of analysis and algorithms for the solution of large-scale systems arising from the discretizations of partial differential equations constrained optimization problems including domain decomposition methods, multilevel methods, and Krylov subspace methods, parallel performance. The aim of this minisymposium is to bring together scientists working in this field to report recent developments in the academic research, as well as in real life engineering applications.

On Schwarz-type smoothers for saddle-point problems with applications to PDE-constrained optimization problems. **Rene Simon** (Universität Linz, Austria), Walter Zulehner (Universität Linz, Austria) IC/MT2146/061

In this talk we consider additive (and multiplicative) Schwarz-type iteration methods for saddle point problems as smoothers in a multigrid method. Each iteration step requires the solution of several small local saddle point problems. In a previous work (by Joachim Schöberl and Walter Zulehner) the general construction of such patch smoothers for mixed problems were discussed. It was shown that, under suitable conditions, the additive Schwarz-type iteration fulfills the so-called smoothing property, an important part of a multigrid convergence proof, and the theory was applied to the Stokes problem. Here we consider a certain class of optimization problems from optimal control. A natural property of the corresponding Karush-Kuhn-Tucker (KKT) system, a 2-by-2 block system which characterizes the solution of the optimization problems, is the positivity of the (1,1) block only on the kernel of the (2,1) block. We extend the results for the Stokes problem to PDE-contrained optimization problems and present a patch smoother, which allows a rigorous convergence analysis of the corresponding multigrid method.

Computing bounds to exact outputs of PoissonŠs equation. **Marius Paraschivoiu** (Concordia University, Canada), Shahin Ghomeshi (Concordia University, Canada), Zhong Cheng (Concordia University, Canada) IC/MT2428/061

In this work we describe a method for obtaining rigorous upper and lower bounds to an output of the exact solution of the three-dimensional Poisson problem. The basic approach stems from the two-level residual based technique where the global problem is decomposed into independent local elemental subproblems by relaxing the continuity along the edges of a triangular partitioning of the entire domain, using approximate Lagrange multipliers. The method then exploits the Lagrangian saddle point property by recasting the output problem as a constrained minimization problem, and the constraints are the modified finite element equilibrium equations and the inter subdomain continuity requirements. An augmented Lagrangian is then constructed, which includes the output and the constraints as part of its formulation and the objective is then a quadratic error formulation of the desired output to be minimized. The gradient condition of the Lagrangian, then leads to four discrete problems: the primal-adjoint pair and two equilibration equations which yield the Lagrange multipliers due to the constraints. More recently, bounds to the exact outputs of interest have been obtained for the Poisson equation, the advection-diffusion-reaction equation, and the linear elasticity equation. However, the results presented were restricted to two-dimensions. The new ingredients in this work are two-fold: first, the finite element tearing and interconnecting (FETI) is invoked in order to calculate the inter-subdomain continuity multipliers (hybrid fluxes) and then extend the approach to three-space dimensions where we present bounds to the exact output of interest in a cube geometry. Secondly, the computational cost in computing the primal-adjoint pair of equations is addressed by using the FETI procedure in the calculations of the elemental subdomain solutions, which thus avoids the need for these global calculations.

Approximation of the Hessian for large-scale optimal-design problems. **Eyal Arian** (Boeing, Seattle, USA) IC/MT2588/061

In the area of aerodynamic design optimization second order derivatives are required to achieve accurate optimal solutions. These are not available in the current technology at Boeing (TRANAIR) since their computation requires unaffordable computing resources. Instead low rank quasi-Newton methods are used that build the Hessian using an update strategy which is not sufficient to achieve tight convergence given the available resources. Our interest is in developing a different method to approximate the Hessian that involves the exploitation of the structure imposed by the governing partial differential equations, and has the potential of improving the convergence of aerodynamic design optimization by orders of magnitude. In this talk a summary of the latest developments in this area will be presented.

IC/MP1050/043: Preconditioned iterative methods for PDE constrained optimization. #2

Organiser: Marcus Sarkis (WPI/USA and IMPA/Brazil)
Co-organiser: Xiao-Chuan Cai (University of Colorado at Boulder, USA)

(For abstract, see session #1 above.)

Fully-coupled domain-decomposition methods for inverse elliptic problems. **Xiao-Chuan Cai** (University of Colorado at Boulder, USA) IC/MT2526/061

In this talk we discuss a class of parallel full space Lagrange–Newton–Krylov–Schwarz (LNKSz) algorithms for inverse elliptic problems. In LNKSz, a Lagrangian functional is first formed according to the inverse elliptic problem with a proper regularization, and then differentiated to obtain an optimality system of nonlinear equations. Inexact Newton's method with line search is then applied directly to the fully coupled nonlinear optimality system and at each Newton's iteration the Jacobian system is solved with a Krylov subspace method preconditioned with an overlapping additive Schwarz method. We apply LNKSz to some parameter identification problems described as minimization problems constrained by elliptic partial differential equations. We report some promising results of a PETSc based parallel implementation of LNKSz for several different types of inverse problems. This is a joint work with S. Liu and J. Zou.

An optimal preconditioner for a class of distributed control PDE constrained optimization problems. **Sue Dollar** (Rutherford Appleton Laboratory, UK), Tyrone Rees (University of Oxford, UK), Andy Wathen (University of Oxford, UK) IC/MT1655/061

The nature of the quadratic sub-problems within PDE-constrained optimization problems means that iterative methods are frequently used to solve the resulting saddle-point systems of the form

$$\begin{bmatrix} A & B^T \\ B & 0 \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix} = \begin{bmatrix} b \\ d \end{bmatrix}.$$

Constraint preconditioners have shown much promise in the context of using iterative methods for solving many of the saddle-point problems that arise from finite dimensional optimization problems. By considering a class of distributed control PDE constrained optimization problems, we will show that various constraint preconditioners can be used with these problems. Significantly, applying the preconditioning step within an interative method requires only solves with diagonal matrices *and* the preconditioners are optimal: typically only a few PPCG iterations are required for the various problems we have considered.

Reconstruction of 3D distributed parameter functions with discontinuities. **Uri Ascher** (University of British Columbia, Canada) IC/MT1614/061

We consider inverse problems of shape recovery from noisy boundary data, where the forward problem involves the inversion of elliptic PDEs. The piecewise constant solution, a scaling and translation of a characteristic function, is described in terms of a smoother level set function. We have recently proposed a fast and robust dynamic regularization method for this purpose.

For problems of moderate size in two spatial variables, direct linear algebra methods have been found rather effective. For larger problems, especially in three spatial variables, iterative methods are required. Perhaps contrary to initial intuition, the iterative methods are particularly useful for the inverse rather than the forward linear systems. Preconditioned CG is investigated and the efficacy of the obtained method is demonstrated.

Joint work with K. van den Doel

IC/MP3827/061: Optimization for systems governed by partial differential equations.

Organiser: Chunming Wang (University of Southern California, USA)
Co-organiser: Gary Rosen (University of Southern California, USA)
Co-organiser: Gunther Peichl (Universität Graz, Austria)

The mathematical theory and computational techniques for the optimization of systems governed by partial differential equations and other infinite dimensional systems have become increasingly relevant in a host of engineering and scientific applications including atmospheric and geophysical data assimilation, weather modeling and forecasting, flow control, nanophotonic and quantum electronic device design, and optimal design for advance materials manufacturing. In many of these application areas, development of mathematical approaches play a key role in the advancement of both the technology and the science. In addition to the numerical solution of the underlying partial differential equations and resulting nonlinear programming problems that are fundamental to these applications, there are also a significant number of other mathematical challenges that are common to optimal control, estimation and design problems. These challenges include dimensionality explosion for many estimation and design problems, nonconvexity of objective functions, computational challenges resulting from the need for efficient and highly accurate evaluation of derivatives, to name just a few. The field of optimal control, estimation and design for distributed parameter systems has seen great expansion in recent years with the growth of the readily availability of advanced and high performance computational resources. This has resulted in significant and important technological advances in many application areas. The synergistic relationship between distinct and diverse applications has the potential to lead to breakthroughs in many more areas of scientific research and engineering development. The speakers in this session represent a large cross-section of the community of mathematicians working in this important area of applied mathematics. Their presentations showcase their successes in developing, using, and analyzing wide ranging mathematical theory and computational methods to solve control, estimation and design problems in the context of a variety of applications involving partial differential equations at the frontier of scientific and engineering research.

Shape-optimization/fictitious-domain approach for numerical realization of a class of free-boundary problems. **Jaroslav Haslinger** (Univerzita Karlova, Czech Republic) IC/MT3808/061

A moving-boundary problem with kinetic condition: well-posedness of weak solutions and parameter identification issues. **Adrian Muntean** (Universität Bremen, Germany) IC/MT3876/061

We report on new results concerning global existence, uniqueness and stability with respect to data and parameters of weak solutions to a two-phase non-equilibrium moving-boundary system arising in the carbonation of concrete. The main feature of the model is the use of a kinetic condition for driving the interface into the unsaturated reactive porous material. Few issues concerning the identification of some diffusion rates as well as the identification of the moving boundary are also addressed.

IC/MP146/061: Optimal control, estimation, and design for systems governed by partial differential equations: theory and computational methods.

Organiser: Chunming Wang (University of Southern California, USA)
Co-organiser: Gunther Peichl (Universität Graz, Austria)
Co-organiser: Gary Rosen (University of Southern California, USA)

The mathematical theory of, and computational methods for the optimal control, estimation and design of systems governed by partial differential equations have become increasingly relevant in a host of engineering and scientific applications including atmospheric and geophysical data assimilation, weather modeling and forecasting, flow control, nano-photonic and quantum electronic device design, and optimal design for advance materials manufacturing. In many of these application areas, development of mathematical approaches play a key role in the advancement of both the technology and the science. In addition to the numerical solution of the underlying partial differential equations and resulting nonlinear programming problems that are fundamental to these applications, there are also a significant number of other mathematical challenges that are common to optimal control, estimation and design problems. These challenges include dimensionality explosion for many estimation and design problems, nonconvexity of objective functions, computational challenges resulting from the need for efficient and highly accurate evaluation of derivatives, to name just a few. The field of optimal control, estimation and design for distributed parameter systems has seen great expansion in recent years with the growth of the readily availability of advanced and high performance computational resources. This has resulted in significant and important technological advances in many application areas. The synergistic relationship between distinct and diverse applications has the potential to lead to breakthroughs in many more areas of scientific research and engineering development. The speakers in this session represent a large cross-section of the community of mathematicians working in this important area of applied mathematics. Their presentations showcase their successes in developing, using, and analyzing wide ranging mathematical theory and computational methods to solve control, estimation and design problems in the context of a variety of applications involving partial differential equations at the frontier of scientific and engineering research.

Variational approach to shape derivatives. **Gunther Peichl** (Universität Graz, Austria) IC/MT1186/061

A general framework for calculating shape derivatives for optimization problems with partial differential equations as constraints is presented. The proposed technique allows to obtain the shape derivative of the cost without the necessity to involve the shape derivative of the state variable. In fact, the state variable is only required to be Lipschitz continuous with respect to the geometry perturbations. Applications to inverse interface problems, and shape optimization for elliptic systems are given.

A level-set method for a shape optimization problem in induction heating processes. **Rachid Touzani** (Université Clermont-Ferrand, France), Anis Kooli (Universite Blaise Pascal, Clermont-Ferrand, France) IC/MT1823/061

We consider, in this presentation, a coupled elliptic–parabolic problem involved in electromagnetic induction processes. In order to design efficient inducting devices, we formulate a topological shape optimization problem. The problem is solved by using a level set formulation. Using the material derivative technique, we derive the gradient expression of the objective function and formulate a level set equation. Numerical simulations demonstrate the efficiency of the numerical method.

Design and optimization of quantum systems. **Russel Caflisch** (University of California, Los Angeles, USA) IC/MT2071/061

This talk will describe the simulation, design and optimization of quantum systems. The examples are a qubit for use in quantum communication or quantum computation and a layered device designed to give a desired electron transmission probability. In the first example, the qubit is realized as the spin of a single trapped electron in a semi-conductor quantum dot. The quantum dot and a quantum wire are formed by the combination of quantum wells and gates. The design goal for this system is a "double pinchoff", in which there is a single trapped electron in the dot and a single (or small number of) conduction states in the wire. Because of considerable experimental uncertainty in the system parameters, the optimal design should be "robust", in the sense that it is far away from unsuccessful designs. We use a Poisson-Schrödinger model for the electrostatic potential and electron wave function and a semi-analytic solution of this model. Through a Monte Carlo search, aided by an analysis of singular points on the design boundary, we find successful designs and optimize them to achieve maximal robustness. In the second example, the stoichiometry of the layers are chosen to best match the desired transmission probability. These values are optimized using a multiscale random search, in which a coarse grained model is used to find the basins of attraction, and a find scale model is used to get to the bottom of the basins.

Mathematical approach for optimal design of electromagnetic and photonic devices. **Chunming Wang** (University of Southern California, USA), Anthony Levi (University of Southern California, USA), Philip Seliger (University of Southern California, USA) IC/MT516/061

Optimal design of photonic devices is a crucial step in the application of nano-technology. In these design problems the number of design parameters is often very large. The multitude of phyiscal constrains severely limit the designers' ability to use their intuition to obtain optimal designs. Mathematical system theory and optimization technique offer considerable promise for assisting designers of these devices. In this presentation, we discuss the objective and formulation of a design problem of electro-magnetic wave-guide using dielectric scattering materials. This design problem is used as a prototype design problem for photonic device design because the physics of this problem can be scaled to photonic device size. An adjoint method based optimization technique is used for the search of locally optimal designs. The modeling and the design approach is validated by carefully constructed laboratory experiments. The significant agreement between optimal design derived by the design software and the experimental results demonstrates the power of the optimal design approach. We shall also present in this talk our attempts in addressing sensitivity and robustness of the optimal designs.

IC/MP146/061: Optimal control, estimation, and design for systems governed by partial differential equations: theory and computational methods. #2

Organiser: Chunming Wang (University of Southern California, USA)
Co-organiser: Gunther Peichl (Universität Graz, Austria)
Co-organiser: Gary Rosen (University of Southern California, USA)

(For abstract, see session #1 above.)

Generalized sensitivity analysis in a delay system. **Franz Kappel** (Universität Graz, Austria) IC/MT995/061

In contrast to classical sensitivity which describes the dependence of a model output on parameters, generalized sensitivity is a measure for the sensitivity of estimated parameters against measurements. In the talk we generalize this concept for delay systems.

Two-scale models for corrosion of porous media . **Sebastian Meier** (Universität Bremen, Germany), Michael Böhm (Universität Bremen, Germany) IC/MT1006/061

Reactive transport in porous media is governed by at least two highly different spatial scales: the *pore scale* and the *macroscopic scale*, the latter of which is usually of interest in applications. For special classes of problems it has been shown by periodic homogenisation that two-scale models are appropriate, in which local transport and reaction as well as their influence on the evolving pore structure are described by local cell problems. A highly important industrial application is the chemical degradation of concrete structures via carbonation. Compared to classical averaged models, such two-scale models involve additional parameters describing the pore geometry (and its evolution!) that have to be identified.

We consider in detail the forward modelling problem leading to a system of parabolic PDEs and ODEs. Moreover, we indicate some relevant parameter identification problems. Due to the non-standard coupling of the equations, the setup of these problems seems to be rather intricate.

Deconvolving blood-alcohol concentration and alcoholic beverage consumption from biosensor measurements of transdermal alcohol. **Gary Rosen** (University of Southern California, USA), Miguel Dumett (University of Southern California, USA), Yuliya Piterbarg (University of Southern California, USA), Alan Schumitzky (University of Southern California, USA) IC/MT985/061

We consider the problem of determining blood alcohol concentration (BAC) and/or the quantity of alcohol consumed (CA) by a subject from biosensor observations of the amount of alcohol excreted through the skin via perspiration. Our approach involves the forward modeling of the transport of ethanol from ingestion, into the blood, through the skin and to the electrochemical sensor where it is processed and its quantity is recoded. The model consists of a system of coupled ordinary and partial differential equations. Once the physiological parameters in the model have been estimated, determining BAC and CA may be formulated as deconvolution problems where the underlying convolution kernel is the impulse response function for an infinite dimensional system. In this talk we will present and discuss our results for estimating the kernels, and the BAC and CA signals from actual patient data. In particular, we will discuss schemes that have allowed us to estimate the kernels deterministically with minimal patient data and statistically for entire populations of subjects. We will also discuss a method for deconvolving the CA signal in the form of an impulse train via a technique based on trigonometric moments that has been used in the sequencing of DNA.

Numerical solution of the free boundary Bernoulli problem. **François Bouchon** (Université Clermont-Ferrand, France), Stéphane Clain (Université Paul Sabatier Toulouse III, France), Rachid Touzani (Université Clermont-Ferrand, France) IC/MT1087/061

We present an iterative method to solve the Bernoulli problem. The scheme uses a perturbation technique to build a sequence of boundaries which converges to the solution of the problem. The boundaries are described by level set functions, which need to be calculated on the whole computational domain. The velocity of the interface is evaluated on the free boundary by solving an elliptic problem, using an immersed interface technic. A Fast marching method is then used both to extend the velocity on the computational domain, and to reinitialize the level set as the signed distance function. Numerical tests are presented to show the efficiency of the method.

IC/MP305/062: Stabilization and control for PDEs of interest to the applied sciences.

Organiser: Piermarco Cannarsa (Università degli Studi di Roma Tor Vergata, Italy)
Co-organiser: Fatiha Alabau Boussouira (Universite Paul Verlaine Metz, France)
Co-organiser: Judith Vancostenoble (Universite Toulouse III, France)

Partial Differential Equations (in short, PDEs) are widely acknowledged as an essential tool to study a large variety of applied systems, from physics to engineering, from biology to economics. Human actions on these systems, to drive them to a desired state or minimize a cost or a time of realization for a given state is an essential aim for engineering applications. This leads to the study of the so-called stabilization and control problems for PDEs.

On the one hand, one may want to use a controller to steer a given system to a prescribed configuration in finite time, or at least get close to it (exact and approximate controllability, respectively), or else converge asymptotically to a given configuration as $t \to \infty$ (stabilization). On the other hand, one may be interested in using controllers to optimize a given performance criterion or cost functional (optimal control). Both kind of problems are also important for equations including nonlocal terms, as this allows to model memory terms of interest to material science, in particular viscoelastic materials.

Stabilization and control problems for PDEs have been intensively studied over the last few decades under the pressure of such a rapidly increasing range of applications. New important ideas and techniques have been developed during the last five years or so to attack problems that had been reckoned as almost impossible to treat, such as Navier–Stokes equations, fluid–structure interaction, degenerate problems. Moreover, some of the techniques developed for a specific purpose turned out to be useful in completely different kinds of context, such as Carleman estimates that are relevant for controllability as well as inverse problems.

This minisymposium aims at illustrating some of the latest and most important achievements of the research in the above area, comparing different approaches and trying to single out possible new connections among them. Special focus will be devoted to PDE models that are relevant to material sciences, population genetics, fluid dynamics and aerodynamic shape optimization. Some presentations will be mainly concerned with the qualitative analysis of the model, others will rather dicuss numerical results.

Some controllability problems of evolution equations. **Oleg Emanouilov** (Colorado State University, USA) IC/MT2561/062

We discuss some recent results in the global exact boundary controllability of evolution equations such as the Navier–Stokes system, the Korteweg–de Vries equation, the cubic Shrödinger equation.

Observability time and semi-discretization. **Paola Loreti** (Universita' degli Studi di Roma "La Sapienza", Italy) IC/MT1208/062

The harmonic analysis method is a good tool to get rather precise estimates of the observability time for linear evolutionary partial differential equations. Our approach is based on a classical theorem due to Ingham [1].

In our talk first we recall well-known results in the continuous case. Then we present some recent theorems on semi-discretization. The new results we discuss were obtained in collaboration with V. Komornik[3] and M. Mehrenberger[5].

[1] Ingham, A.E.; Some trigonometrical inequalities with applications in the theory of series. Math. Z. 41 (1936), pp.367–379.

[2] Komornik, V. and Loreti, P.; *Fourier Series in Control Theory*, Springer, New York 2005.

[3] Komornik, V. and Loreti, P.; Semi-discrete Ingham type inequalities, accepted for publication in the special issue of Applied Mathematics and Optimization on New Developments in the Control of PDE, with Applications.

[4] Loreti, P.; On some gap theorems. European women in mathematics—Marseille 2003, 39–45, CWI Tract, 135, Centrum Wisk. Inform., Amsterdam, 2005.

[5] Loreti, P. and Mehrenberger, M.; An Ingham type proof for a two-grid observability theorem. (submitted).

Carleman estimates for degenerate parabolic equations. **Patrick Martinez** (Universite Paul Sabatier Toulouse III, France), Piermarco Cannarsa (Università degli Studi di Roma Tor Vergata, Italy), Judith Vancostenoble (Universite Toulouse III, France) IC/MT2507/062

We study the controllability properties of parabolic equations degenerating at the boundary of the space domain.

We derive new Carleman estimates for the degenerate parabolic equation

$$w_t + (a(x)w_x)_x = f, \quad (t,x) \in (0,T) \times (0,1),$$

where the function a mainly satisfies

$$a \in C^0([0,1]) \cap C^1((0,1)),\ a > 0 \text{ on } (0,1) \text{ and } \frac{1}{\sqrt{a}} \in L^1(0,1).$$

We are mainly interested in the situation of a degenerate equation at the boundary i.e. in the case where $a(0) = 0$ and/or $a(1) = 0$. A typical example is $a(x) = x^\alpha(1-x)^\beta$ with $\alpha, \beta \in [0,2)$.

As a consequence, we deduce null controllability results for the degenerate one dimensional heat equation

$$u_t - (a(x)u_x)_x = h\chi_\omega, \quad (t,x) \in (0,T)\times(0,1), \quad \omega \subset\subset (0,1).$$

IC/MP305/062: Stabilization and control for PDEs of interest to the applied sciences. #2

Organiser: Piermarco Cannarsa (Università degli Studi di Roma Tor Vergata, Italy)
Co-organiser: Fatiha Alabau Boussouira (Universite Paul Verlaine Metz, France)
Co-organiser: Judith Vancostenoble (Universite Toulouse III, France)

(For abstract, see session #1 above.)

Stabilization of the 2D Navier–Stokes equations by finite-dimensional controllers. **Jean-Pierre Raymond** (Université Paul Sabatier Toulouse III, France) IC/MT1887/062

We are interested in the boundary feedback stabilization of the incompressible Navier–Stokes equations, by a finite dimensional feedback controller, about an unstable stationary solution. Such stabilization problems have been recently studied with controls belonging to infinite dimensional spaces. Here we shall present two local stabilization results. In the first one, the feedback control is obtained by solving a control problem for an infinite dimensional system (even if the control is of finite dimension). In the second one, the feedback control is obtained by solving a control problem of finite dimension.

Remarks on the control of Euler and Navier–Stokes equations with applications to optimal shape design in aeronautics. **Francisco Palacios** (Instituto Nacional de Técnica Aeroespacial, Spain), Enrique Zuazua (Universidad Autónoma de Madrid, Spain), Carlos Castro (Universidad Politécnica de Madrid, Spain), Carlos Lozano (Instituto Nacional de Técnica Aeroespacial, Spain) IC/MT2031/062

In the present work we will address several issues concerning adjoint-based shape optimization problems in aeronautics. The key issue here is to obtain the sensitivity or gradient of a certain cost function under shape deformations. Adjoint techniques allow to dramatically reduce the computational cost of the procedure. Our aim, apart from swiftly reviewing the continuous adjoint methodology for the calculation of shape sensitivities, is to shed light on the discrete vs. continuous adjoint dichotomy, placing the emphasis on the well-posedness of the approaches, distinguishing between two independent issues which are normally mixed up in the literature: non-differentiability of numerical schemes and non-regular field solutions.

In practical design applications one works with numerical approximation of the flow equations, so the discrete adjoint method appears to be the natural approach. However, efficient numeric schemes are often non-differentiable and, consequently, the cost function depends on the solution and on the design parameters in a non-differentiable way. In a strict sense, it is therefore impossible to build gradient-based descent algorithms upon such schemes. To make things work in practice several tricks are used whose validity has to be carefully assessed. On the other hand, the continuous adjoint approach constitutes an alternative that allows to maintain the rigor throughout the whole procedure. However, in continuous schemes flow discontinuities may arise. In this case, shocks must be treated as singularities on which adjoint Rankine-Hugoniot conditions must be enforced.

We end by commenting on the application of the Level Set method to aeronautical design. The Level Set method is a numerical technique for tracking interfaces and shapes which, when suitably interpreted in the aeronautical design context, provides great versatility when working in cases where great changes in shape topology are either expected or desirable.

Stabilization for visco-elastic materials: abstract results and applications. **Fatiha Alabau Boussouira** (Universite Paul Verlaine Metz, France) IC/MT2469/062

We study visco-elastic materials for which the feedback law is of memory type, that is the feedback appears as a convolution operator with respect to time. We prove stabilization properties such as exponential or polynomial decay for general abstract hyperbolic equations with applications to various models.

About the vibration of a beam between two stops. **Jaime Muñoz Rivera** (Laboratório Nacional de Computação Científica, Brazil) IC/MT2041/062

We consider the vibration model of a thermoelastic beam with two transversal obstacles. The corresponding mathematical model is a variational inequality of fourth order. We show that there exist at least one solution which decay exponentially to zero. We also show that the solution of the variational inequality has smoothing effect property over the initial data. The uniqueness is an open question.

IC/MP321/062: Control of deterministic systems under state constraints.

Organiser: Hélène Frankowska (École Polytechnique, France)
Co-organiser: Piermarco Cannarsa (Università degli Studi di Roma Tor Vergata, Italy)

Constrained systems arise in different models of applied sciences (drug administration, robotics, aeronautics, chemistry, environmental sciences and many others). In recent years substantial progress was done in control theory for deterministic systems under general state constraints. In the past, a typical way to handle constraints was based on penalisation methods, which may be heavy to handle numerically and are usually less informative. Recently, direct methods were developed which helped to prove simultaneously necessary optimality conditions, their nondegeneracy and normality, and also to investigate the non occurrence of the Lavrentieff phenomenon for such models. This also allowed to develop the theory of second order optimality conditions, and obtain perimeter and volume estimates for the reachable set of state-constrained controlled system. Another important progress was done in sensitivity analysis and the extensions of Hamilton–Jacobi theory to constrained deterministic systems. The aim of this minisymposium is to give an overview of these recent advances and new methods.

Second-order conditions in stability analysis for state-constrained optimal-control problems. **Kazimierz Malanowski** (Polish Academy of Sciences, Poland) IC/MT1295/062

In stability analysis for optimization problems conditions are investigated, under which the solutions and Lagrange multipliers are locally Lipschitz continuous with respect to parameters. The methodolgy, based on Robinson's implicit function theorem for generalized equations, allows to reduce the stability analysis for nonlinear cone constrained optimization problems, to such an analysis for linear-quadratic accessory problems. Applying this methodology to nonlinear optimal control problems, we have to analyse stability of the solutions to linear-quadratic accessory optimal control problems, with respect to additive perturbations. In getting stability results for this class of problems, two types of assumptions are crucial: constraint qualifications and coercivity conditions. These conditions should be stable in a neighborhood of the reference point.

Clearly, we would like to have the assumptions as weak as possible. For control-constrained problems, a full characterization of the stability property is known. The situation is different for

state-constrained problems, where a strong coercivity condition has been used. The reason was the difficulty with proving stability of the weakened coercivity condition.

In the present talk, it will be shown that the second order conditions, weakened by taking into account the strongly active state constraints, are stable under small perturbations. The proof of this stability property, takes advantage of a mechanism, different from that used in the case of control constraints. The above result allows to obtain stability results for state-constrained optimal control problems, under assumptions weaker than those known from the literature.

On necessary conditions for state-constrained problems. **Maria Margarida Ferreira** (Universidade do Porto, Portugal), Maria do Rosário de Pinho (Universidade do Porto, Portugal) IC/MT2479/062

This work focuses on necessary conditions for weak local minimizers of optimal control problems with state constraints. More precisely the addressed problem is to minimize:

$$g(x(0),x(1)) + \int_0^1 L(t,x(t),u(t))\mathrm{d}t$$

subject to $\dot{x}(t) = f(t,x(t),u(t))$ and $h(t,x(t)) \leq 0$, with $u(t) \in U(t)$ and $(x(0),x(1)) \in C$.

For a weak local minimizer $(\bar{x},\bar{u})$ the non smooth maximum principle asserts, among other conditions, that

$$-\dot{p}(t) \in \operatorname{co} \partial_x H(t,\bar{x}(t),\bar{u}(t),q(t),\lambda) \quad \text{a.e.}$$
$$\max_{u\in U(t)} H(t,\bar{x}(t),u,q(t),\lambda) = H(t,\bar{x}(t),\bar{u}(t),q(t),\lambda) \quad \text{a.e.}$$

where p is an absolutely continuous function, q is a function of bounded variation, $\lambda \geq 0$ is a scalar and H is the Hamiltonian:

$$H(t,x,u,p,\lambda) = p \cdot f(t,x,u) - \lambda L(t,x,u)\,.$$

We derive in this work a nonequivalent necessary condition:

$$(-\dot{p}(t),\xi(t)) \in \operatorname{co} \partial_{x,u} H(t,\bar{x}(t),q(t),\bar{u}(t))\,, \quad \xi(t) \in \operatorname{co} N_{U(t)}(\bar{u}(t)) \quad \text{a.e.}$$

Non-degenerate necessary conditions for nonlinear optimal-control problems with higher-index state constraints. **Fernando Fontes** (Universidade do Minho, Portugal), Sofia Lopes (Universidade do Minho, Portugal) IC/MT3123/062

For some optimal control problems with pathwise state constraints the standard versions of the necessary conditions of optimality are unable to provide useful information to select minimizers. There exist some literature on stronger forms of the maximum principle, the so-called nondegenerate necessary conditions, that can be informative for those problems. These conditions can be applied when certain constraint qualifications are satisfied. However, when the state constraints have higher index (i.e. their first derivative with respect to time does not depend on the control) these nondegenerate necessary conditions cannot be used. This happens because constraint qualifications assumptions are never satisfied for higher index state constraints.

We note that control problems with higher index state constraints arise frequently in practice. An example is a common mechanical systems for which there is a constraint on the position (an obstacle in the path, for example) and the control acts as a second derivative of the position (a force or acceleration) which is a typical case.

Here, we provide a nondegenerate form of the necessary conditions that can be applied to nonlinear problems with higher index state constraints. When addressing a problem with a state constraint of index k, the result described is applicable under a constraint qualification that involves the k-th derivative of the state constraint, corresponding to the first time when derivative depends explicitly on the control.

Holder continuity of adjoint states and optimal controls for state constrained problems. **Hélène Frankowska** (École Polytechnique, France), Piernicola Bettiol (SISSA, Trieste, Italy) IC/MT1400/062

This talk is devoted to Hölder regularity of adjoint states and optimal controls for the Bolza optimal control problem under state constraints, where the goal is to minimize the functional

$$J(x,u) := \varphi(x(0),x(1)) + \int_0^1 \ell(t,x(t),u(t))\,dt$$

over all absolutely continuous $x(\cdot)$ and measurable $u(\cdot)$ satisfying

$$x'(t) = f(t,x(t),u(t)),\ u(t) \in U(t),\ x(t) \in K\ \forall\ t \in [0,1],\ (x(0),x(1)) \in K,$$

The associated Hamiltonian is defined by

$$H(t,x,p) = \sup_{u\in U(t)} \{\langle p, f(t,x,u)\rangle - \ell(t,x,u)\}.$$

Consider any optimal solution satisfying the normal constrained maximum principle and let $N_K(x)$ denote the normal cone to K at x. We show that whenever H is smooth and monotone in the directions normal to constraints, in the sense that for some $k > 0$ and $\beta \geq 1$

$$\begin{cases} \forall\ (t,x) \in [0,1]\times K \ \text{ and } \ \forall\ p,q \in R^n \ \text{ with } \ p-q \in N_K(x) \\ \left\langle \frac{\partial H}{\partial p}(t,x,p) - \frac{\partial H}{\partial p}(t,x,q), p-q \right\rangle \geq k|p-q|^{1+\beta}, \end{cases}$$

then both the adjoint state of the maximum principle and the derivative of this optimal trajectory are Hölder continuous for smooth constraints, while they are both side lower Hölder continuous for less regular constraints. Finally, we provide sufficient conditions for Hölder type regularity of optimal controls.

IC/MP321/062: Control of deterministic systems under state constraints. #2

Organiser: Hélène Frankowska (École Polytechnique, France)
Co-organiser: Piermarco Cannarsa (Università degli Studi di Roma Tor Vergata, Italy)

(For abstract, see session #1 above.)

Regularity of reachable sets under state constraints. **Pierre Cardaliaguet** (Université Brest, France) IC/MT1462/062

Recently the regularity problem of reachable sets for controls systems has attracted a lot of attention: in particular bounds on the size of the boundary has been used to investigate existence and uniqueness of solutions for some models of dislocation dynamics. Similar questions for control systems under state constraints turn out to be much more delicate. In this joint work with C. Marchi, we explain how to handle the problem in dimension 2.

An HJB approach for a deterministic state-constraint optimal-control problem without controllability assumption. **Olivier Bokanowski** (Université Pierre et Marie Curie, France) IC/MT3188/062

We study the optimal (deterministic) control problem with state constraints, without any particular controllability assumption. We are interested by the characterization of the value function as the lower semi-continuous viscosity solution of some Hamilton-Jacobi-Bellman equation.

Several results have been obtained in this direction, leading to the existence and uniqueness in the form of a PDE. In general either an inward constraint qualification (such as Soner's qualification's constraint [1]), or an outward constraint qualification (such as in Frankowska and Vinter [2]) is assumed. On the other hand, a characterization without qualification constraint is also obtained in Ref. [3], using a Viability approach.

In our approach, we give a PDE-like characterization. We use the concept of contingent epiderivatives as in [2], and also a new type of condition on the border of the constraint set. Known results using inward or outward qualification constraints can then be interpreted in this framework.

Motivated by the preliminary numerical work [4], we shall also propose a numerical procedure based on our theoretical results.

This is a joint work with N. Megdich and H. Zidani (UMA, Ensta, France).

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[2] H. Frankowska and R. B. Vinter, J. Optim. Theory Appl., Vol 104(1), 21-40 (2000).

[3] P. Cardaliaguet, M. Quincampoix and P. Saint-Pierre, Appl. Math. Optim. Vol 36, 21-42 (1997).

[4] O. Bokanowski, S. Martin, R. Munos and H. Zidani, Appl. Num. Math. Vol. 56 (9), 135-1254 (2006).

Lipschitz continuity of solutions to Bolza optimal-control problems. **Elsa Maria Marchini** (Università degli studi di Milano-Bicocca, Italy) IC/MT2734/062

We investigate Lipschitz continuity of optimal solutions for the Bolza optimal control problem which consists in minimizing the functional

$$\int_0^T L(t,x(t),u(t))dt + g(x(0),x(T))$$

over all trajectory/control pairs (x,u) subject to the state equation

$$\begin{cases} x'(t) = f(t,x(t),u(t)) & \text{for a.e. } t \in I \\ u(t) \in U(t) & \text{for a.e. } t \in I \\ x(t) \in K & \text{for every } t \in I \\ (x(0),x(T)) \in Q, \end{cases}$$

with suitable assumptions on data. Since our result on regularity is a consequence of normal necessary conditions for optimality, we propose new sufficient conditions for normality of state-constrained non smooth maximum principles for absolutely continuous optimal trajectories.

Existence and regularity of solutions to Bolza problems with slow growth. **Piermarco Cannarsa** (Università degli Studi di Roma Tor Vergata, Italy) IC/MT2169/062

The existence and Lipschitz continuity of optimal trajectories for the Bolza problem is a classical topic in control theory. To study such a problem, the Lagrangian is usually assumed to possess superlinear growth at infinity in the control variables. In this paper, building on a work by Clarke for the calculus of variations, we provide sufficient conditions in Hamiltonian form for the existence and regularity of solutions to nonlinear optimal control problems with state constraints, relaxing the fast growth condition for the Lagrangian.

IC/MP244/063: Interior-point methods for model predictive control.

Organiser: Moritz Diehl (Katholieke Universiteit Leuven, Belgium)
Co-organiser: Steve Wright (University of Wisconsin, USA)

Model predictive control (MPC) is an advanced feedback control technique that requires the reliable solution of a sequence of optimization problems in real-time. One of the major reasons for its success in practice is its ability to deal with inequality constraints on controls and internal system states, which cannot be treated by most other existing feedback control techniques. The availability of reliable quadratic programming solvers based on active set strategies was a crucial factor in making the success of MPC since the 1980s possible, and active set methods are still used in many MPC applications.

On the other hand, tremendous progress has been made in the last decade in the optimization community in developing interior point methods for problems with large numbers of inequality constraints. Thus, when MPC optimization problems with several thousand inequality constraints shall be solved, interior point methods are often superior to active set methods. However, one of the main drawbacks of interior point methods for MPC can be seen in their limited warm starting capabilities, which are important in MPC, where a sequence of only slowly changing optimization problems are solved. This drawback limits the application of interior point methods in particular to fast MPC applications.

Aim of the minisymposium is to bring together two groups of people: on the one hand, control engineers that have successfully developed or used interior point methods for MPC optimization, and on the other hand numerical optimizers that are distinguished by their work on warm starting capabilities for interior point methods. The possible results of the minisymposium are unexpected contacts of people and ideas that shall help to advance the development of faster, practically applicable interior point methods for model predictive control.

Interior-point methods in MPC: a survey. **Steve Wright** (University of Wisconsin, USA), Moritz Diehl (Katholieke Universiteit Leuven, Belgium) IC/MT3393/063

We introduce this minisymposium by surveying the use of interior-point methods in model predictive control (MPC) to date. We discuss both linear and nonlinear MPC, and discuss the pros and cons relative to alternative approaches. We also discuss warm starting issues in interior-point methods, which are particularly relevant to MPC, as well as recently proposed applications to robust control.

Unblocking heuristics for warm-starting interior-point methods. **Andreas Grothey** (University of Edinburgh, UK) IC/MT2399/063

Warmstarting Interior Point Methods is difficult. Unlike the situation in the simplex method, an Interior Point warmstart might not be any better than a coldstart and can even lead to worse performance. A common observation with "failed" warmstarts are blocking directions: after a warmstart only very small steps can be made. We will address the question of how to find a good warmstarting point. Further we will present experience with a set of new heuristics targeted at directly unblocking the current step, resulting in better and more reliable warmstarts. We will present results on the Netlib test set as well as on a selection of large scale nonlinear problems.

A path-following method for parametric nonlinear complementarity problems. **Martin Weiser** (Zuse-Institut Berlin, Germany), Roland Griesse (RICAM Linz, Austria), Moritz Diehl (Katholieke Universiteit Leuven, Belgium) IC/MT1586/063

The talk presents an algorithmic framework based on regularized complementarity functions for approximately solving parametric nonlinear complementarity problems as they arise in particular in nonlinear model predictive control. The aim is to select step sizes and regularization such that an inexact pathfollowing scheme limited to one Newton correction per step is able to reliably follow the parameter-dependent solution. Features of the approach are discussed on the basis of several numerical examples.

A continuation/GMRES method for real-time algorithm of constrained nonlinear-model predictive control. **Toshiyuki Ohtsuka** (Osaka University, Japan), Yuichi Shimizu (Osaka University, Japan), Moritz Diehl (Katholieke Universiteit Leuven, Belgium) IC/MT1825/063

This talk gives an overview of a continuation-based real-time algorithm for nonlinear model predictive control. The optimal solution is updated by solving a linear equation only once at each sampling time, and the linear equation can be solved efficiently with a Krylov subspace method, GMRES. In addition to the basic idea of the algorithm, implementation examples for mechanical systems are presented with emphasis on practical handling of inequality constraints. These are treated by the introduction of penalized slack variables in a way that bears some similarity to interior point methods with a fixed barrier parameter.

IC/MP244/063: Interior-point methods for model predictive control. #2

Organiser: Moritz Diehl (Katholieke Universiteit Leuven, Belgium)
Co-organiser: Steve Wright (University of Wisconsin, USA)

(For abstract, see session #1 above.)

A sensitivity-based barrier strategy for nonlinear-model predictive control. **Lorenz Biegler** (Carnegie Mellon University, USA), Victor Zavala (Carnegie Mellon University, USA) IC/MT2497/063

In less than two decades, Nonlinear Model Predictive Control (NMPC) has evolved from a conceptual framework to a tractable and well-demonstrated approach for the control of constrained nonlinear processes. These advances have been realized both through better understanding of stablity and robustness properties, as well as improved nonlinear programming (NLP) formulations and algorithms for dynamic optimization. This talk further reduces the on-line computational expense for NMPC through the development of a sensitivity-based formulation consisting of the following steps:

- A large, sparse NLP is formulated through a total discretization of the moving horizon problem.
- The discretized NMPC problem is solved in background using a fast barrier NLP method.
- As new state information is received, the NLP solution is immediately updated on-line using a sensitivity-based formulation derived from the barrier method.

Our initial tests indicate that the on-line computational expense for NMPC can be reduced by about two orders of magnitude with little sacrifice in performance. This talk discusses important elements of this procedure. Moreover, further refinements are presented that include experiences with warm start strategies and the examination of nominal and robust stability properties for this NMPC strategy.

Model predictive control under probability distributions. **Marc Steinbach** (Leibniz Universität Hannover, Germany) IC/MT2545/063

We consider model predictive control under the assumption that random disturbances result from a stochastic process with known probability distribution. A dynamic stochastic programming approach is proposed to achieve optimal performance on average while ensuring that later disturbances can always be corrected. We present a suitable interior point method for solving the resulting large structured optimization problems, and algorithmic aspects regarding computational complexity are discussed. A continuously operating distillation process with a feed tank buffering uncertain inflows serves to illustrate the approach. We study a simple linear-quadratic stochastic tracking model and an integrated model with differential-algebraic equations as dynamic constraints in the stochastic program. Computational results will be presented.

Conic programming formulations for robust MPC. **Moritz Diehl** (Katholieke Universiteit Leuven, Belgium) IC/MT1091/063

In this talk we treat the robust min-max model predictive control (MPC) formulation for linearly constrained polytopic systems with quadratic cost, and show that it can be cast as a specific conic program, namely a quadratically constrained quadratic program (QCQP). To derive this result, we use the rigorous closed loop formulation of min-max MPC, and show that any such min-max MPC problem with convex costs and constraints can be cast as a finite dimensional convex optimization problem, with the QCQP arising from quadratic costs as a special case. At the base of the proof is a lemma showing the convexity of the dynamic programming cost-to-go, which implies that the worst case on an infinite polytopic set is assumed on one of its finitely many vertices. As the approach is based on a scenario tree formulation, the number of variables in this problem grows exponentially with the horizon length. Fortunately, the QCQP is tree structured, and can thus be efficiently solved by specially tailored interior-point methods whose computational costs are linear in the number of variables. The new formulation as a tree sparse QCQP thus promises to facilitate the online solution of the rigorous min-max MPC problem with quadratic costs.

Efficient robust optimization for robust control with constraints. **Eric Kerrigan** (Imperial College London, UK), Paul Goulart (University of Cambridge, UK) IC/MT1587/063

In this talk we present an efficient computational technique for the optimal control of linear discrete-time systems subject to bounded disturbances and linear constraints on the states and inputs. The problem of computing an optimal state feedback control policy over a finite horizon, given the current state, is nonconvex. A recent breakthrough has been the application of robust optimization techniques to reparameterize this problem as a convex program. While the reparameterized problem is theoretically tractable, the number of variables is quadratic in the horizon length and has no apparent exploitable structure. We focus on the situation when the disturbance set is norm bounded and the cost function to be minimized is quadratic in the states and inputs. In this case a sparse problem structure can be recovered via introduction of state-like variables and decomposition of the problem into a set of coupled finite horizon control problems. This decomposed problem can then be formulated as a highly structured quadratic program, solvable by a primal-dual interior-point method for which each iteration requires a number of operations that increases cubicly with the horizon length. This cubic iteration time can be guaranteed using a standard Riccati-based block factorization technique from discrete-time optimal control. Numerical results will be presented, using a standard sparse primal-dual interior point solver, that illustrate the efficiency of this approach.

IC/MP291/063: Geometric optimisation in linear algebra, signal processing and control.

Organiser: Knut Hüper (NICTA, Australia)
Co-organiser: Uwe Helmke (Julius-Maximilians-Universität Würzburg, Germany)

This minisymposium focuses on geometrically constrained optimisation tasks, with a wide range of applications in systems and control, numerical linear algebra, signal processing, computer vision and statistics. Recently, differential geometric ideas have been combined with nonlinear optimisation methods to solve complicated and highly non-convex optimisation tasks, thus enabling one to tackle advanced engineering applications that cannot be easily approached using more standard convex or unconstrained optimisation ideas. The minisymposium will meet the challenge of providing efficient mathematical tools for geometrically structured optimisation problems by bringing together leading experts in this quickly growing area. Current research in this field is focused on

(i) development of convergence results

(ii) generalisations to non-Riemannian settings

(iii) investigations on new application areas.

All three directions will be represented, thus allowing a broad overview on recent developments.

Optimization algorithms for computing numerical ranges and the tensor SVD. **Gunther Dirr** (Julius-Maximilians-Universität Würzburg, Germany), Uwe Helmke (Julius-Maximilians-Universität Würzburg, Germany), Oana Morar (Universität Würzburg, Germany) IC/MT1999/063

A number of interesting computational problems in linear algebra and quantum computing can be formulated as the task of optimizing trace functions on unitary orbits of elements in a tensor product of complex vector spaces. Explicitly, we consider the linear action of certain subgroups K of the unitary group $U(n)$, acting on the complex Hilbert space $H := \mathbb{C}^{n_1} \otimes \cdots \otimes \mathbb{C}^{n_r}$, $n = n_1 + \cdots + n_r$ in the natural way. For any two elements $c, a \in H$ we study the geometry of the subset

$$W_K(c,a) := \{\langle c, g \cdot a\rangle | g \in K\}$$

of the complex plane. The set $W_K(c,a)$ is a generalization of the C-numerical range from operator theory. It also connects to quantum computing and the tensor SVD – an efficient tool for data compression in pattern recognition. These connections will be outlined in the talk. Geometric optimization algorithms for maximizing the real part function $z \mapsto \mathrm{Re}(z)$ on $W_K(c,a)$ are developed.

Vector transport on manifolds. **Pierre-Antoine Absil** (Université Catholique de Louvain, Belgium), Robert Mahony (Australian National University), Rodolphe Sepulchre (Université de Liège, Belgium) IC/MT297/063

We consider the problem of finding an extremum of a smooth real-valued function on a smooth manifold where Hessian information is not available. Several optimization algorithms on Euclidean space (such as quasi-Newton and conjugate gradient methods) achieve superlinear convergence without making use of the Hessian of the cost function. These algorithms gather second-order information on the cost function by *comparing* gradient vectors at various neighboring points. To generalize this idea on smooth manifolds, one must overcome the difficulty that the gradient vectors at two different points of the manifold belong to two different tangent spaces and cannot be compared directly. When the manifold is endowed with an affine connection, the classical remedy is to use parallel translation to move one of the tangent vectors along a geodesic between the two points. However, computing parallel translation requires the solution of a set of ordinary differential equations that rarely has a closed-form solution and may be as computationally challenging as the original optimization problem.

In this work, we define sufficient properties for a generalization of the parallel translation, called *vector transport*. We show that in superlinear optimization algorithms on manifolds, parallel translation can be replaced by any vector transport without affecting the superlinear convergence. We also give examples of vector transports that are algebraically and computationally simpler than the parallel translation for a number of problems of practical interest. In conclusion, the notion of vector transport makes it possible alleviate the computational burden associated with comparing tangent vectors at various points of a manifold, without compromising the convergence properties of the optimization scheme.

A Newton–Stiefel method using the Cayley transformation. **Paul Van Dooren** (Universite Catholique de Louvain, Belgium), Catherine Fraikin (Universite Catholique de Louvain, Belgium), Knut Hüper (NICTA, Australia) IC/MT378/063

We present a parameterization of the Stiefel manifold that allows to perform a Newton step (constrained to the Stiefel manifold) in a relatively simple manner. The parameterization is based on the Cayley transformation which maps skew symmetric matrices into orthogonal matrices. We then apply this technique to a problem occurring in the analysis of graphs [1].

We also illustrate the local quadratic convergence of this method using examples coming from [1].

Reference

[1] C. Fraikin, Yu. Nesterov and P. Van Dooren, Optimizing the coupling between two isometric projections of matrices, submitted to Siam J. Matr. Anal. and Appl., 2005.

FastICA, Rayleigh-quotient iteration and some generalisations. **Knut Hüper** (NICTA, Australia) IC/MT1942/063

One of the state of the art algorithms for linear Independent Component Analysis in Signal Processing is FastICA, developed by the Finnish school. This very efficient algorithm enjoys nice interpretations similar to the socalled Rayleigh-Quotient-Iteration (RQI) well known to the Numerical Linear Algebra community. It can be considered as an optimisation procedure on a manifold related to intrinsic Newton-type iterations. We will discuss some of the known facts of FastICA and then present more recent results towards parallel implementations and better convergence properties.

IC/MP685/063: Symbolic and numerical computations for convex analysis.

Organiser: Yves Lucet (University of British Columbia, Canada)

Convex optimization is a fundamental branch of optimization. It provides a suitable framework from both a theoretical and a practical point of view for many problems, classical (such as image reconstruction) and contemporary (such as semidefinite programming). In this minisymposium, the speakers will discuss convex optimization problems and associated objects from a computational point of view. The algorithms presented will include purely symbolic algorithms using modern computer algebra systems, numerical algorithms adapted from computational geometry, hybrid symbolic–numeric algorithms, and optimization algorithms tailored to the numerical computation of specific convex objects.

The authors will focus on a class of functions that allows hybrid symbolic–numeric computations of convex transforms; on the symbolic computation of Fenchel conjugates; on the numerical computation of the cone of autocorrelated components; and on new principle in medical imaging called thermo-acoustic tomography.

Hybrid symbolic–numeric algorithms for computational convex analysis. **Yves Lucet** (University of British Columbia, Canada) IC/MT686/063

Computational convex analysis focuses on developing efficient tools to compute fundamental transforms arising in convex analysis. Symbolic computation tools have been developed, and have allowed more insight into the calculation of the Fenchel conjugate and related transforms. When such tools are not applicable e.g. when there is no closed form, fast transform algorithms perform numerical computation efficiently.

However, all fast transform algorithms rely on discretizations of the input and output functions, where the accuracy of the approximation is at best first-order. Moreover, they do not allow to easily compose several transforms. On the contrary, we consider the class of piecewise linear-quadratic functions which, being closed under the most relevant operations in convex analysis, allows the robust numerical computation of compositions of transforms such as the recently investigated proximal average. The algorithms presented are hybrid symbolic-numeric: they first compute a piecewise-linear quadratic approximation of the function, and then manipulate the approximation symbolically, thereby allowing a robust convex calculus.

Starting from the drawbacks of fast algorithms, we will introduce the class of piecewise-linear quadratic functions along with efficient algorithms to manipulate such functions.

Work done in collaboration with H. Bauschke and M. Trienis.

A fully-nonlinear partial differential equation for the convex envelope. **Adam Oberman** (Simon Fraser University, Canada) IC/MT5021/063

In this talk we introduce a new fully nonlinear Partial Differential Equation for the Convex Envelope of a given function. The equation is in the form of an obstacle problem, where the obstacle is the given function, and the PDE involved the smallest eigenvalue of the Hessian. The equation is useful for computing convex envelopes. Computational examples will be given. It also allows for a stochastic control interpretation for the convex envelope.

Some facts about the cone of vectors with autocorrelated components. **Marc Fuentes** (Université Paul Sabatier Toulouse III, France) IC/MT1320/063

In signal processing and communications, some optimization problems naturally involve the cone of *vectors with autocorrelated components* (also called *finite autocorrelation sequences*). A vector $x = (x_0, x_1, \cdots, x_n) \in \mathbb{R}^{n+1}$ is said to have autocorrelated components if there exists a vector $y = (y_0, y_1, \cdots, y_n) \in \mathbb{R}^{n+1}$ such that

$$x_k = \sum_{i=0}^{n-k} y_i\, y_{i+k} \quad \text{for all } k = 0, \cdots, n\,.$$

Surprisingly enough, this cone turns out to be convex (even if there is no direct simple proof of this property). In the present work, we pursue the works by L. Vandenberghe *et al.* in studying more thoroughly this cone (facets, extreme points, acuteness) and presenting algorithms to project a vector on it; One first effective approach to compute the projection uses interior point methods involving the polar cone. We propose here a non-convex relaxation to overcome the problem of dimensionality inherent to interior point methods and enable us to treat problems of larger size. We will also discuss about the extension in the bidimensionnal case, which can have some applications in image processing.

Mathematics involved in such an approach are: convex analysis and optimization, Toeplitz matrices, Riesz–Féjer representation theorem and trigonometric polynomials.

[1] Alkire, B. and Vanderberghe, L.; Convex Optimization problems involving finite autocorrelation sequences. Mathematical Programming **93**, (2002), pp.331–359.

[2] Fuentes, M.; Analyse Convexe et Optimisation sur le Cône des Vecteurs à Composantes Autocorrélées. Technical Report, Université Paul Sabatier, Toulouse (2005).

Perspectives in various notions of convexity. **Pierre Marechal** (Université Paul Sabatier Toulouse III, France) IC/MT1720/063

Any finite, separately convex, positively homogeneous function on $\Re^2$ is convex. This was first established by Dacorogna. We give a new and concise proof of this result, and we show that it fails in higher dimension. The key of the new proof is the notion of *perspective* of a convex function f, namely, the function $(x, y) \to y f(x/y)$, $y > 0$. In recent works by Maréchal, the perspective has been substantially generalized by considering functions of the form $(x, y) \to g(y) f(x/g(y))$, with suitable assumptions on g. Here, this *generalized perspective* is shown to be a powerful tool for the analysis of convexity properties of parametrized families of matrix functions.

IC/MP63/063: Robust optimization.

Organiser: Kurt Marti (Universität der Bundeswehr München, Germany)
Co-organiser: Volker Schulz (Universität Trier, Germany)
Co-organiser: Thomas Vietor (Ford Werke, Köln, Germany)

In Robust Optimization only partial information is known about the model parameters. This must be taken into account in order to reach optimal decisions/designs which are the least sensitive with respect to parameter variations in the known range of the model parameters. Hence, the original optimization problem with unknown parameters must be replaced by an appropriate deterministic substitute problem incorporating the given information about the parameters. Using decision theoretical principles, substitute problems may be obtained, depending on the available information about the type of uncertainty; e.g., by using minimax- or expectation-operators. Typical substitute problems demand then the minimization of the maximum or expected total costs (initial plus recourse costs) subject to remaining (mostly simple) design constraints, or the minimization of a (simple) cost function subject to reliability constraints involving the probability of structural/system failure/survival. Hence, a first goal of this Minisymposium is to present actual methods for coping with several types of uncertainty in order to get *robust*, hence, most parameter-insensitive optimal decisions/designs. On the other hand, since material, model and design parameters have a stochastic character, in many application areas the importance of the stochastic modelling have been accepted more and more.

Increased demand for robust optimization methods arises in many technical/industrial areas like aerospace development, passenger vehicle engineering, railway engineering, construction of ships. Thus, the second objective of this Minisymposium is to support the exchange between different areas with theoretical and practical focus. This will contribute to an extended view in application areas which includes stochastic modelling and optimization. Furthermore the demands of application areas are formulated and communicated to areas with more theoretical background. This Minisymposium continues a series of Minisymposia on design methods under stochastic uncertainty organized within GAMM.

Stochastic quadratic programming techniques for finding robust optimal designs of plastic mechanical structures. **Kurt Marti** (Universität der Bundeswehr München, Germany) IC/MT1229/063

Problems from plastic analysis and optimal plastic design are based on the convex, linear or linearized yield/strenght condition and the linear equilibrium equation for the stress (state) vector. In practice, one has to take into account stochastic variations of the model parameters (e.g. yield stresses, plastic capacities, external load factors, cost factors, etc.). Hence, in order to get robust optimal load factors, robust optimal designs, resp., the basic plastic analysis or optimal plastic design problem with random parameters must be replaced by an appropriate deterministic substitute problem. Instead of calculating approximatively the probability of failure/survival based on a certain choice of (approximate) failure modes, a direct approach is proposed based on the primary costs (weight, volume, costs of construction, costs for missing carrying capacity, etc.) and the recourse costs (e.g. costs for repair, compensation for weakness within the strucutre, damage, failure, etc.). Based on the mechanical survival conditions of plasticity theory, a quadratic error/loss criterion is developed. The minimum recourse costs can be determined then by solving an optimization problem having a quadratic objective function and linear constraints. For each vector a of model parameters and each design vector x, one obtains then an explicit representation of the "best" internal load distribution F*. Moreover, also the expected recourse costs can be determined explicitly. Consequently an explicit finite dimensional parameter optimization problem results for finding a robust optimal design x*. The analytical properties of the resulting problem are discussed, and applications, such as limit load/shakedown analysis, are considered.

Optimal design of frames under stochastic uncertainties. **Simone Zier** (Universität der Bundeswehr München, Germany) IC/MT1882/063

Structural optimization is an interesting area on which lots of research has already been done. Using the first collapse-theorem the necessary and sufficient constraints of a structure consist of the yield condition and the equilibrium condition. In the recent field of research stochastic uncertainties has been taken into account. This leads to a stochastic optimization problem which cannot be solved using the traditional methods. Instead of that appropriate (deterministic) substitute problems must be formulated.

In the following the design of frames is treated where the load is supposed to be stochastic. Here both forces and moments have to be taken into consideration. The recourse problem will be formulated in general and in the standard form of stochastic linear programming (SLP). Since the original problem is not a linear one, it is necessary to make some approximations and assumptions. After the formulation of the stochastic optimization problem the recourse problem with discretization and the expected value problem are introduced as representatives of substitute problems. Subsequently, optimization results using these methods for the robust optimal design of a storey-frame are presented.

Optimal control of robots under stochastic uncertainty: robust feedback controls. **Michael Schacher** (Universität der Bundeswehr München, Germany) IC/MT1878/063

The most important aspect in the optimal control and design of manipulators is the determination of the basic movement, i.e. the calculation of the optimal trajectory on which the robot has to move. Having an optimal reference trajectory and an optimal open-loop control, there is the need of control corrections by applying a certain feedback control. Different attempts exist for this.

In this presentation a method will be shown which is based on classical control theory, that works with cost functions being minimized. The aim is to take into account stochastic parameter varations in order to obtain robust optimal feedback controls.

After Taylor expansion to calculate expected cost functions and a few transformations it is possible to find an appropriate deterministic substitute control problem: Retaining only linear terms, approximation of expectations and variances of the expected cost function can be obtained. Furthermore, it is necessary to discretisize the objective function and the differential equations. This is handled by means of Splines.

Using stochastic optimization methods, random parameter variations can be incorporated into the optimal control process. Hence, robust optimal feedback controls are obtained.

Variation methods and discrete optimization principles in lattice geometry. **Vladimir Kobelev** (Universität Siegen, Germany) IC/MT3267/063

The contemporary knowledge about the robust discrete optimization is basically restricted to the direct numerical solution of the integer optimization problems. In the present talk we try to establish the theoretical foundation for the discrete optimization and introduce the basic variation principles of lattice geometry. The lattice geometry is essentially the based on quantum calculus of V. Kac and P. Cheung. The objects of lattice geometry - metric tensor, tangent vectors, connections, curvature tensor - appears similar to the corresponding objects of classical differential geometry, but differ from them in some important aspects. The principles of variational lattice calculus are derived. The application of lattice geometry to the robust optimization of discrete geometrical structures is discussed.

IC/MP63/063: Robust optimization. #2

Organiser: Kurt Marti (Universität der Bundeswehr München, Germany)
Co-organiser: Volker Schulz (Universität Trier, Germany)
Co-organiser: Thomas Vietor (Ford Werke, Köln, Germany)

(For abstract, see session #1 above.)

Different methods for robust design and stochastic optimization in vehicle engineering. **Thomas Vietor** (Ford Werke, Köln, Germany) IC/MT1150/063

The development of a passenger car is a multidisciplinary task. The vehicle has to fulfill demands out of different technical attributes beside non-technical requirements like styling and costs. Very often demands out of these areas are conflicting. One main problem is the variability of mechanical quantities responsible for the performance and customer perception of a car. To overcome this, the extension of the conventional deterministic oriented development process to a process which includes stochastic quantities is necessary. In this presentation the current deterministic approach is described briefly. In a first extended version of the process the variability of material parameters is included. In further steps the formulation and solution of stochastic optimization problems for sub-problems are necessary. Finally the complete approach should fully integrate the variability of stochastic quantities.
As extension to already published papers from the same authors in this presentation different approaches to robust design and stochastic optimization are compared. In this comparison well known-methods like first order second moment approaches are included as well as the use of simple Monte-Carlo simulations. Based on the complexity and effort of the different structural analysis methods for different attributes and the number of required function calls a suitable method can be selected. The comparison is extended to selected commercial software packages. For industrial applications commercial software is normally preferred because of the robustness of the software, the well designed user-interface, good documentation and the offered support. In this presentation the authors will investigate the theoretical background of some of the offered commercial software programs and study if they can be applied to real-world examples.

Work done together with Simon van den Akker and Esben Lindgaard Olesen.

Reliability-based optimization using a decoupling approach and reliability sensitivity. **Marcos Valdebenito** (Universität Innsbruck, Austria), Gerhart Schuëller (Universität Innsbruck, Austria) IC/MT2261/063

Reliability-based optimization (RBO) is a challenging task that, on one hand, involves the estimation of the reliability of a structure with respect to a certain limit state considering the uncertainty in loading and/or structural properties. On the other hand, it also involves the solution of an optimization problem. This usually requires a large number of reliability estimations in order to find a design that better fulfills the design requirements (constraints) and minimizes a certain objective function. Analytical solutions for the reliability problem are quite limited; generally it is necessary to apply simulation techniques, which are numerically expensive though. Although significant progress has been achieved recently in the latter field and now reliability analyses can be performed for large structures involving many uncertain parameters, the computational efforts involved in simulation procedures is still considerable. Hence this contribution analyzes the use of approximate measures of the reliability sensitivity (derivatives of the failure probability with respect to the design parameters) which are calculated using the information generated at the reliability estimation stage. The approximate reliability sensitivities, calculated based on the concepts proposed in [1], is combined with a decoupling approach, developed in [2] and further studied in [3], in order to reduce the numerical costs involved in the RBO problem. Examples are shown in order to discuss the advantages and drawbacks of the implemented method.

[1] Wu, Y.T.; Computational Methods for Efficient Structural Reliability and Reliability Sensitivity Analysis. AIAA Journal, 32(8), 1994, pp.1717–1723.
[2] Gasser, M., Schuëller, G.I.; Reliability-Based Optimization of Structural Systems. Math. Methods Oper. Res., 1997, 46, pp.281–307.
[3] Jensen, H.A.; Design and Sensitivity Analysis of Dynamical Systems subjected to Stochastic Loading. Computers & Structures, 83, 2005, pp.1062–1075.

Stochastic programming in financial and energy markets. **Marc Steinbach** (Leibniz Universität Hannover, Germany) IC/MT2918/063

Robustness in the context of trading strategies often means optimal long-term performance (repeated decisions) or mean-risk optimization (one-time decisions), leading to possibly nonlinear multistage stochastic programs. We discuss applications in financial and energy markets and present interior-point based solution algorithms that can be adapted to the specific problem structure. Computational results illustrate the stochastic models and the efficiency of our solution approach.

Avoidance of random obstacles by means of probabilistic constraints. **René Henrion** (WIAS Berlin, Germany) IC/MT2116/063

Obstacle avoidance is an important issue in manufacturing processes or robotics. If only imprecise information is available, it makes sense to understand the obstacle as a random object. Modeling the avoidance of such random obstacles can be done in various ways, the most reasonable of which seems to consist in the formulation of probabilistic constraints. The talk presents shortest path models for pointwise and uniform probabilistic constraints in the case of both the obstacle and the manoeuvrable body being finite unions of convex polytopes. Solution approaches are discussed for the special case of multivariate normal data for the obstacle position in the configuration space. The methods require fast calculation of normal probabilities of polytopes (or equivalently: singular normal distributions). We apply a method based on an inclusion/exclusion formula which allows efficiently to calculate these probabilities along with their gradients with respect to moving position.

IC/MP704/063: Optimal control and stability analysis in dynamical systems, involving parameters.

Organiser: Mihai-Emilian Popescu (ISMMA-Bucharest, Romania)

We consider affine controlled systems:

$$\dot{x} = Y(x(t)) + \sum_{i=1}^{m} X_i(x(t)), \quad x(0) = x_0$$

where $u = (u_1, ..., u_m) \in U = L^2([0,T], \mathbb{R}^m)$. Applications are as follows.

1) Optimal problem: determine the minimum of functionals $J(u) = \int_0^T ah(x_u(t)) + b\varphi(X_u) + \frac{1}{2}cg(X_u)$, with $X_u = Y(x_u) + \sum_{i=1}^m X_i(x_u)$. Here x_u is the integral curve of X_u with origin x_0 and final point x_1. This optimum problem minimizes the totally energy with constraints to be tangentially at affine distribution.
2) The objective of this study is the determination a sweep solution for the class of quadratic functionals with constraints represented by quasi-linear controlled systems with a small parameters. Out of necessary conditions of extremum resulted from the vanishing of the first order differential of the extremized functional, we shall determine to zeroth order solution which corresponds to small parameter equal zero.

The solutions of the systems in variations of the necessary conditions of extremum represents the first-order solution for small parameter different of zero. An approximate solution is obtained as the sum of the zeroth- and first-order solutions.

For a stability analysis, we consider the dynamical system: $\dot{x} = f(x,p)$, where $p \in P \subset \mathbb{R}^k$ is the space parameters which can be varied in system.

A solution $\Phi_\xi : [0,\infty) \to X$ (the state space) of the system (4) with initial point $\xi \in X$ ($\Phi_\xi(0) = \xi$ is called *asymptotically* stable if:

a) $\{\Phi_\xi(t) | t > 0\}$ is bounded (with respect to a norm $\|\cdot\|$ on X;
b) there is a $\varepsilon > 0$ such that for each solution Φ_ξ with $\|\xi - \xi'\| \le \varepsilon$, we have that $\lim_{t\to\infty} \|\Phi_\xi(t) - \Phi_{\xi'}(t^*)\| = 0$.

The time function $t^* : \mathbb{R}_+ \to \mathbb{R}_+$ is defined by

$$\|\Phi_\xi(t) - \Phi_{\xi'}(t^*)\| = \min\{\|\Phi_\xi(t) - \Phi_{\xi'}(t')\| | t' > 0\}.$$

For $t = t^*$ the system is called Liapunov-stable, and the value ε is a measure of the stability of Φ_ξ.

The ball $K(\xi) = \{\xi \in X | \|\xi - \xi'\| < \varepsilon\}$ represents a domain of attraction of a stable solution Φ_ξ. $K(\xi)$ is an open set, therefore $\Phi_{\xi'}$ is also a stable solution for all $\xi' \in K(\xi)$, probably with another measure ε' of stability.

Applications of this method include:

1) One obtains the method for analysis the stability in the class of considered dynamical system.
2) Stability and performance of discrete time residual generators. This study presents a new design method for discrete time residual generators. The fault detection problem is formulated in terms of H_2 and H_∞-type optimization.

Weight-function method in stability study. **Ion Stroe** (Politehnica University of Bucharest, Romania) IC/MT945/063

A new method for systems stability analysis is presented. This method is called weight functions method and it replaces the problem of Liapunov function finding with a problem of finding a number of functions (weight functions) equal to the number of first order differential equations describing the system. It is known that there are not general methods for finding Liapunov functions. The weight functions method is simpler than the classical method since one function at a time has to found. This methodŠs conditions of solution stability for linear and nonlinear systems are presented and holonomic systems with dependent variables are analysed.

Stability and robustness properties for a class of discrete-time residual generators. **Adrian-Mihail Stoica** (Universitatea Tehnică Bucarest, Romania) IC/MT1026/063

The paper presents a new design methodology for residual generators with observer-based structure for which fault detection and disturbance attenuation conditions are determined. The developments are based on H_2 and H_∞ optimisation methods in the discrete-time framework and the solvability conditions are expressed in terms of an appropriate system of matrix inequalities. An important advantage of the proposed approach is that it can be easily extended to other classes of systems (stochastic systems, sampled-data systems, etc.) for which disturbance attenuation type results are available. Robustness properties with respect to parametric uncertainty are also analysed. The theoretical results are illustrated by a case study concerning the Global Positioning System (GPS) integrity monitoring.

Optimal control for quasi-linear systems with small parameters. **Mihai-Emilian Popescu** (ISMMA-Bucharest, Romania) IC/MT1072/063

The objective of this study is the determination of the solution for Bolza problems of optimum from the class of quadratic functionals. The differential restrictions are represented by quasi-linear controlled systems with a small parameter.

Out of necessary conditions of extremum resulted from vanishing of the first order differential of the extremized functional, we shall determine the zeroth order solutions which corresponds to small parameter, $\varepsilon = 0$.

The solution of the system in variations for the necessary conditions of extremum represents the first order solutions for $\varepsilon \neq 0$.

The obtained approximate solution is the sum of the zeroth and first order solutions.

An important result is that on the admissible trajectory $\delta x_0 = 0$ we have variation of adjoint variable, $\delta\lambda_0 \neq 0$ and, hence, the variation δu of the control on the extremal is different from zero. This correspond to the fact that the admissible trajectory is a neighboring optimal trajectory.

Thus, the first order solution is the neighboring optimal trajectory for a given value of the small parameter.

In the previously treated cases, the admissible trajectory could not be a neighboring optimal trajectory, the property we have stated being satisfied only for the analyzed case of the nonlinear systems with a small parameter.

A method for optimal control in boundary-layer flow. **Alexandru Dumitrache** (ISMMA - Bucharest, Romania) IC/MT3084/063

In this paper is presented a methodology for active flow control which couples the time-dependent Navier–Stokes system with an adjoint Navier–Stokes system and optimality conditions from which unsteady flow fields and controls (e.g., actuators), may be determined. The problem of boundary layer instability suppression through wave cancellation is used as the initial validation case to test the methodology.

The objective of control is to match the stress vector along a portion of the boundary to a given vector; instability suppression is achieved by choosing the given vector to be that of a steady base flow. Control is realized through the injection or suction of fluid through a single oriffice on the boundary. The present method may be applied to separation control, relaminarization, and turbulence control applications.

IC/MP273/063: Recent advances in derivative-free optimization.

Organiser: Virginia Torczon (College of William and Mary, USA)
Co-organiser: Robert Lewis (College of William and Mary, USA)

The optimization of complex systems often involves simulation codes for which either derivatives have not been provided or approximations of derivatives are problematic. Furthermore, the computational costs associated with the simulations can be appreciable. Recent research efforts in derivative-free optimization have focused on effective algorithmic techniques for challenges such as handling general nonlinear constraints, approximating curvature information, and distributing the computing. The aim of this minisymposium is to report both the theoretical and computational advances made in these arenas.

Sparsity of the average-curvature information matrix. **Trond Steihaug** (University of Bergen, Norway), Lennart Frimannslund (Universitetet i Bergen, Norway) IC/MT2174/063

The class of Generating Set Search (GSS) Methods is a large class within derivative free optimization methods. We present a GSS method which uses average curvature to generate the search directions. If the function that is minimized is smooth then the average curvature will be a good approximation to the Hessian matrix (and exact for quadratic functions)

Some functions are expensive to evaluate accurately, but cheap to evaluate approximately. The approximated function can be regarded as the original function subject to numerical noise and the function will be non-smooth. We show that partial separability properties can still be exploited in the context of an optimization method although the original function is distorted by noise. We show this by introducing the covariation graph of the variables which may be derived from a data dependency graph. The average curvature can be computed efficiently using information about the covariation graph.

In the context of computing the curvature information matrix, we encounter a subproblem of selecting rows from a matrix, where the number of rows is much greater than the number of columns, to obtain a full rank and well-conditioned matrix with minimum effort. Finding the optimal solution to this problem is an open problem. We present an efficient heuristic solution.

The theoretical framework we use for computing the curvature information matrix can also be used for approximating Hessians in other derivative free optimization methods.

This is joint work with Lennart Frimannslund, Department of Informatics,University of Bergen.

Sequential penalty derivative-free methods for nonlinear constrained optimization. **Giampaolo Liuzzi** (Università degli Studi di Roma "La Sapienza", Italy), Stefano Lucidi (Università degli Studi di Roma "La Sapienza", Italy), Marco Sciandrone (Università degli Studi di Firenze, Italy) IC/MT1436/063

We consider the problem of minimizing a continuously differentiable function of several variables subject to smooth nonlinear constraints. We assume that the first order derivatives of the objective function and of the constraints can be neither calculated nor approximated explicitly. This class of problems arises in many industrial and scientific applications and this motivates the increasing interest in the study of derivative-free methods. In this work we propose new globally convergent methods based on smooth sequential penalty functions. Furthermore, we show the numerical results of computational experiments performed on standard test problems.

Augmented Lagrangian generating-set search for solving nonlinear constrained optimization problems. **Virginia Torczon** (College of William and Mary, USA), Robert Lewis (College of William and Mary, USA) IC/MT3155/063

We discuss an augmented Lagrangian approach to applying generating set search to nonlinear programming. The approach is based on the approximate minimization, with a suitable derivative-free stopping criterion, of a sequence of augmented Lagrangian relaxations of the original problem, with bound and general linear constraints kept explicit. We highlight the analytical results underlying the approach and provide numerical illustrations. We also discuss strategies for active set identification and techniques for accelerating the overall optimization process.

An asynchronous parallel derivative-free software package for handling nonlinear constraints. **Joshua Griffin** (Sandia National Laboratories, USA), Tamara Kolda (Sandia National Laboratories, USA) IC/MT5025/063

Many real-life optimization problems present formidable challenges despite having a relatively small number of independent variables. Difficulties can arise from nonsmoothness, discontinuities, and noise. Further, function evaluations typically involves calling unwieldy CPU-intensive simulation software that may periodically crash. In this context, we present a globally convergent derivative-free method for nonlinear programming based on generating set search. Linear constraints are handled using conforming search directions. Several options for handling nonlinear constraints are explored, including an augmented Lagrangian approach. All methods are implemented asynchronously in parallel. We present extensive test results using the CUTEr test set.

IC/MP66/063: Algorithms for nonlinear optimization.

Organiser: Ya-xiang Yuan (Chinese Academy of Sciences)

Research on algorithms for nonlinear optimization is one of the very active research directions in optimization. In recent years there are many researches on large scale nonlinear optimization, special structured optimization problems and new type of algorithms (such as the filter methods and trust-region methods).

Global minimization on quadratic least-squares problems. **Xin Liu** (Chinese Academy of Sciences) IC/MT4369/063

We consider the global minimization on quadratic least squares(QLS) problems, which is a widely used model appearing in various areas such as industry, computational biology and so on. By discussing the properties of the local minima of QLS problems, we present some ideas for solving these problems efficiently.

On projected gradient methods for regularizing reconstruction of synchrotron radiation spectra distribution function. **Yanfei Wang** (Chinese Academy of Sciences) IC/MT2619/063

The theory of synchrotron radiation (SR) has been well-understood and published. We study the numerical methods for the reconstruction of the spectral distribution function of SR by measurement of the attenuation of the SR energy spectrum. The reconstruction of the spectral distribution function of SR is an ill-posed integral operator equation of the first kind. Therefore, how to overcome the ill-posedness is a major task in numerical computation. We study projected gradient meth-

ods for the regularized problem with nonnegative constraints. The feasibility of the method is studied in detail by using a hypothetical SR spectrum. The applied results of the spectrum of 4W1B beamline in BSRF (Beijing Synchrotron Radiation Facility) are shown. Work done in collaboration with Y.Du and T.Hu.

On adaptive step-size selections in gradient methods. **Gaetano Zanghirati** (University of Ferrara, Italy), Giacomo Frassoldati (Modena, Italy), Luca Zanni (Università degli Studi di Modena e Reggio Emilia, Italy) IC/MT2782/063

In recent years a number of different proposals for the selection of the step-size have largely improved the gradient-based methods, in the case of both constrained and unconstrained nonlinear optimization. Many of these proposals aim to achieve a good convergence rate by exploiting the Barzilai-Borwein (BB) step-sizes. To this purpose, several modifications of the original BB idea have been investigated (step-size alternations, cyclic step-sizes, adaptive selections) and have clearly shown their benefits. Motivated by the effectiveness of these modified BB rules, we propose a simple adaptive selection where the standard BB rule is alternated with a new step-size, which gets meaningful convergence rate improvements when compared with other recent BB-like gradient schemes. The actual behavior of the new method is shown on a set of well known test problems, as well as on a real-world application.

Conjugate-gradient methods in Banach spaces. **Ivie Stein** (The University of Toledo, USA) IC/MT2573/063

One purpose of this paper is to extend the conjugate gradient method to minimize functions on Banach Spaces that are norm reflexive and strictly convex. The algorithms in this paper are based upon the notion of the metric gradient defined by Michael Golomb and Richard Tapia (Numer. Math. 20 (1972) 115-124). Generalizations have been made for the algorithms of Daniel, Polak-Ribiere and Fletcher-Reeves. The primary purpose here is to present applications including problems in differential equations and the calculus of variations where the Banach spaces are Sobolev Spaces.

IC/MP66/063: Algorithms for nonlinear optimization. #2

Organiser: Ya-xiang Yuan (Chinese Academy of Sciences)

(For abstract, see session #1 above.)

A trust-region-type regularization of Newton's method. **Coralia Cartis** (Rutherford Appleton Laboratory, UK), Nicholas Gould (University of Oxford, UK), Philippe Toint (FUNDP Namur, Belgium) IC/MT2742/063

A new regularization technique for Newton's method with strong global convergence and good complexity properties was recently proposed (Nesterov & Polyak, 2006). In this, an improved estimate of the solution is computed by finding the global minimizer of a cubic model of the objective function, and there is an obvious connection to trust region methods. We address the challenges of making such an algorithm implementable and computationally efficient. The cubic model may be approximately minimized either explicitly, using a Krylov approach, or implicitly by solving a bi-level univariate minimization problem involving a sequence of trust-region subproblems as a function of their radii. Compared to existing strategies, apart from overall efficiency of this new approach, we are interested in the performance on problems for which NewtonŠs method performs poorly, because of ill-conditioning or singularity.

A new trust-region algorithm for nonlinear constrained optimization. **Niu Lingfeng** (Chinese Academy of Sciences), Ya-xiang Yuan (Chinese Academy of Sciences) IC/MT2325/063

We propose a new trust region algorithm for nonlinear constrained optimization problems. In each iteration of our algorithm, the trial step is computed by minimizing a quadratic approximation to the augmented Lagrangian function in the trust region. Based on the model problem, we give a new Lagrangian multiplier estimation and the corresponding formula for the actual/predicted reduction. A penalty function procedure combing with a new filter technique is used to force convergence when the initial values of the variables are far from the solution. The second order correction technique is utilized to avoid the Maratos effect. We report numerical results for a set of constrained problems from the CUTEr collection. Global convergence and fast local convergence for the test problems are observed.

An affine-scaling interior-point CBB method for box-constrained optimization. **William Hager** (University of Florida, USA), Hongchao Zhang (University of Minnesota, USA) IC/MT2539/063

Our algorithm combines an affine scaling approach with a cyclic Barzilai–Borwein (BB) gradient method. Global convergence is established along with local $\mathbb{R}$-linear convergence at a nondegenerate local minimizer where the second-order sufficient optimality conditions are satisfied. An application is given to penalized maximum likelihood reconstruction in positron emission tomography.

A power–penalty method for a linear complementarity problem. **Xiaoqi Yang** (Hong Kong Polytechnic University, PR China), Song Wang (University of Western Australia) IC/MT2563/063

In this paper we propose a power penalty approach to a linear complementarity problem (LCP). This approach is based on approximating the LCP by a nonlinear equation with a power penalty term. We prove that the solution to the equation converges to that of the LCP at a rate equivalent to the power used in the penalty term when the penalty parameter tends to infinity.

IC/MP5051/063: Algorithms for nonlinear optimization (II).

Organiser: Ya-xiang Yuan (Chinese Academy of Sciences)

Research on algorithms for nonlinear optimization is one of the very active research directions in optimization. In recent years there are many researches on large scale nonlinear optimization, special structured optimization problems and new type of algorithms (such as the filter methods and trust-region methods).

Solving a class of constrained black-box *inverse variational inequalities.* **Bingsheng He** (Nanjing University, PR China) IC/MT4385/063

In some practical applications of equilibrium problems, the status, instead of the variables, is required in a constrained set. The mathematical form of such problems is Find u such that $f(u) \in S$, and $(f' - f(u))^T u \leq 0$, $\forall f' \in S$, where $S = S(f) = \{f \in R^n \mid A^T f = b$ (or $A^T f \leq b)$, $f \in \mathcal{F}\}$. We call such problems inverse variational inequalities (IVI) because the variable and the function are in the opposite positions of the classical one. Usually, the function in IVI arising from real world does not have any explicit forms and we can only evaluate or observe the function value for given variables from some 'black-boxes'. For a class of constrained 'black-box' inverse variational inequalities, we present a proximal point like algorithm (PPA)-based method that only needs the function value for given variables in the solution process.

IC/MP655/064: Dynamics of equilibrium problems via game theory, evolutionary variational inequalities, complementarity and projected dynamical systems.

Organiser: Monica-Gabriela Cojocaru (University of Guelph, Canada)

The interest in modelling applied equilibrium problems (be it via Wardrop and/or Nash equilibria) has been ever increasing in the last decades, with vast ramifications and developments in nonlinear and variational analysis, in particular in the directions of projected dynamical systems, complementarity problems and variational inequalities. Game theory has also undergone a strong development, being intimately related to optimization of network problems, either from the user point of view, or from the system design/service level agreement point of view.

There are exciting theoretical and computational advances in all these areas today, and there is a considerable number of scientists with complementary expertise actively engaged in such research worldwide. This minisymposium explores the interactions among scientists in similar areas of research. It highlights important contributions to building theoretical models and simulations of applied equilibrium problems, ranging from vaccination policies to operations research and economics problems (like transportation, spatial and financial pricing, internet or energy market modelling).

A fast contraction mapping for solving multibody systems. **Alessandro Tasora** (Università degli Studi di Parma, Italy), Mihai Anitescu (Argonne National Laboratory, USA) IC/MT1672/064

The simulation of complex multibody systems with contacts and friction require a fast and robust solver for complementarity problems. This work presents an efficient method which can solve large cone-complementarity problems by means of a fixed point iteration. Our method performs like a contractive mapping, providing a monotonic approximation to the exact solution. The algorithm features high computational performance even if thousands of unilateral constraints are added to the system. Also, this scheme fits well in a real-time simulation context because it can be terminated prematurely. Differently from LCP approaches, nonlinear constraints introduced by friction in three-dimensional space are taken into accounts without using polyhedral approximations. With few modifications, a parallel version of this iterative scheme can be implemented on SIMD computing architectures.

Evaluating the Impact of Average Cost Based Contracts on the Industrial Sector in the European Emission Trading Scheme. **Giorgia Oggioni** (Università di Bergamo, Italy & KU Leuven, Belgium), Yves Smeers (Université Catholique de Louvain, Belgium) IC/MT2740/064

This paper addresses a problem arising from the combination of the restructuring of the European electricity sector and the introduction of the EU Emission Trading System (EU-ETS). Electricity intensive industrial consumers are currently facing a high price of electricity, which endangers their competitiveness and may force them to leave Europe. This would be a serious welfare loss for European countries with possibly non-environmental gain. The decrease of their European emission of CO_2 would indeed have no effect if these industries go and emit CO_2 elsewhere.
We explore the possibility of developing special contracts, which would limit the impact of CO_2 prices on electricity intensive industrial consumers. We first consider a reference situation of a perfectly competitive market where electricity prices are identical for all consumers and based on the short run marginal costs. We, then, recognize that electricity intensive consumers require a different electricity service: the bulk of their demand is indeed long-term and very high load. They are also in a position to finance the construction and the operation of large generation units. We therefore consider an alternative organization whereby electricity intensive industrial consumers pay a price corresponding to the full cost of base load plants.
We conduct a sample analysis on a prototype problem that is meant to represent Northwestern Europe (Belgium, France, Germany and the Netherlands). The models are formulated as complementarity problems and are solved in GAMS using PATH.

Electricity investments in an uncertain environment. **Yves Smeers** (Université Catholique de Louvain, Belgium) IC/MT2922/064

Investments in electricity generation are now facing considerable uncertainties, whether due to restructuring or carbon constraints. Uncertainties make investment more costly and may jeopardize security of supply. Standard minimal cost optimization models that simulate the development of competitive electricity markets in the long term are not really equipped for exploring these questions.
We consider equilibrium models of investment in competitive electricity markets that differ by the underlying representation of uncertainty. A first model assumes competing firms with different costs of capital (CAPM). A second model supposes that the firms are exposed to risk factors with different risk premium (APT). Last, we consider true stochastic equilibrium models with risk adverse firms in competition. We discuss both the formulations of these models and their casting in computable form.

Equilibrium dynamics of group vaccination strategies in a heterogeneous population with a given vaccine coverage profile. **Monica-Gabriela Cojocaru** (University of Guelph, Canada) IC/MT3119/064

We analyze here vaccination strategies games in a heterogeneous population whose individuals are partitioned in groups according to their (distinct) perceived relative risk assessments of vaccination. By relative we mean a ratio between the perceived risk of the vaccine, versus the perceived risk of becoming infected. In order to analyze such problems, we use the theories of variational inequalities and projected dynamical systems, both finite and infinite dimesional. In this work we are interested to track the dynamics of a group's equilibrium vaccination strategy, given that the vaccine coverage in the population as a whole is known. Game theoretical models illustrate how vaccine scares and declining vaccine coverage, especially in countries with voluntary vaccination policies are not isolated historical events, but rather possible instances of inherently unstable dynamics which can apply in any population under a voluntary vaccination policy. While mandatory vaccination would serve the public interest by effectively eradicating diseases, there are also implications for individual rights. Understanding and predicting long-term trends in population vaccination behaviour via game dynamic models is therefore valuable for the development of sound, evidence-based public health policy.

IC/MP655/064: Dynamics of equilibrium problems via game theory, evolutionary variational inequalities, complementarity and projected dynamical systems. #2

Organiser: Monica-Gabriela Cojocaru (University of Guelph, Canada)

(For abstract, see session #1 above.)

Frictional-contact problems with local compliance. **Jong-Shi Pang** (Rensselaer Polytechnic Institute, USA) IC/MT3151/064

A 3-dimensional frictional contact model with local compliance and damping was introduced in the 2002 Ph.D. thesis of Peng Song and was subsequently studied extensively in several papers by Song, Kumar, and Pang. In this work, we examine a variation of this model where there is no damping in the normal contact forces but there is coupled stiffness between the normal and tangential forces via body deformations. We show that this frictional contact model admits a formulation as an ordinary differential equation with a boundedly Lipschitz continuous, albeit implicitly defined, semismooth right-hand side with global linear growth. Several major consequences follow from such a formulation: (a) existence and uniqueness of a continuously differentiable solution trajectory originated from an arbitrary initial state, (b) finite contact forces that are semismooth functions of the system state, (c) semismooth dependence of the trajectory on the initial state, (d) convergence of a shooting method for solving two-point boundary problems, and (e) the absence of Zeno states. The derived results are valid for both a dynamic model and a quasistatic model, the latter being one in which inertia effects are ignored, and for a broad class of "semismoothly regular" friction cones that include the well-known quadratic Coulomb cone and its polygonal approximations.

Convergence of semi-implicit time-stepping schemes for nonsmooth dynamics. **Mihai Anitescu** (Argonne National Laboratory, USA), Florian Potra (National Institute of Standards and Technology, USA) IC/MT3221/064

In this work we present a framework for the convergence analysis in a measure differential inclusion sense of a class of time-stepping schemes for multibody dynamics with contacts, joints, and friction. This class of methods solves one linear complementarity problem per step and contains the semi-implicit Euler method, as well as trapezoidal-like methods. By using the concept of a reduced friction cone, the analysis includes a convergence result for the case that includes joints. An unexpected intermediary result is that we are able to define a discrete velocity function of bounded variation, *although the natural discrete velocity function produced by our algorithm may have unbounded variation*. Several numerical simulations are presented to demonstrate the validity of our findings.

Infinite-dimensional duality theory and applications to network equilibrium models. **Patrizia Daniele** (Università degli Studi di Catania, Italy) IC/MT3547/064

We present an infinite dimensional duality theory for optimization problems and evolutionary variational inequalities where the constraint sets are given by inequalities and equalities.

The difficulties arising from the structure of the constraint set are overcome by means of generalized constraint qualification assumptions based on the concept of quasi relative interior of a convex set.

We also apply such results to a general evolutionary network model, which includes as special cases traffic, spatial price and financial equilibrium problems.

Dynamic oligopolistic market equilibrium problem. **Annamaria Barbagallo** (Università degli Studi di Catania, Italy), Monica-Gabriela Cojocaru (University of Guelph, Canada) IC/MT5028/064

The aim of the talk is to present the oligopolistic market equilibrium problem when the data is dependent on time. We show under which assumptions the existence of the dynamic solution is ensured. We apply the regularity results proved recently in relation to this problem. Then, by means of the continuity of equilibrium solution, we can introduce a method to compute the solutions.

IC/MP295/067: Global optimization applications via SPSA.

Organiser: Rafael Banchs (Universitat Politècnica de Catalunya, Spain)
Co-organiser: Adolfo Rodriguez (University of Texas at Austin, USA)
Co-organiser: Hector Klie (University of Texas at Austin, USA)

Many of the optimization problems encountered in practical engineering and scientific applications have to deal with multiple suboptimal local solutions. In this sense, global optimization methods provide means for finding good global solutions by reducing the risk of being trapped in local solutions. The main problem of global optimization methods is that they are generally very expensive and time-consuming from the computational point of view.

The SPSA (Simultaneous Perturbation Stochastic Approximation) algorithm has lately received considerable attention because its simplicity, flexibility and low computational cost. Indeed, the algorithm only requires one or, at most, two function evaluations per iteration independently of the parameter space size in order to generate a stochastic descent direc-

tion. This constitutes a very convenient feature when dealing with large parameter spaces and/or very complex and time-expensive forward modeling algorithms. SPSA also constitutes a very attractive alternative for global optimization problems where it is unfeasible to compute function gradients.

SPSA performs random simultaneous perturbations of all model parameters to generate a descent direction at each iteration. Despite the random character of the procedure, the expected value of the computed direction is the deterministically steepest descent direction. Only two parameters, which form monotonically decreasing sequences with respect to the iteration index have to be tuned to ensure asymptotic convergence of the algorithm.

This minisymposium focuses on global optimization applications by using SPSA. After an introductory speech about the algorithm itself, some applications of the algorithm in very different engineering and scientific problems, ranging from the oil industry to natural language processing will be presented and discussed.

The magic of SPSA. **László Gerencsér** (Hungarian Academy of Sciences, Hungary), Zsuzsanna Vágó (Pázmány Péter Katolikus Egyetem, Hungary), Stacy Hill (The Johns Hopkins University, USA) IC/MT3195/067

In his seminal 1992 paper, J. Spall introduced the simultaneous perturbation stochastic approximation (SPSA), the prime targeted area being function minimization on heavy terrain: when function evaluation is expensive and noisy and gradients are not available by direct experiments. The main objective of SPSA is to achieve a prescribed accuracy with possibly smallest number of measurements.

The basic idea is a simple, but unlikely observation saying that it is possible to generate an unbiased estimator of the gradient of a quadratic function in any dimension with just two measurements. Indeed, if $f(x)$ is a quadratic function and we define the vector

$$H(x) = \frac{1}{2}(f(x+u) - f(x-u))v$$

where the random vectors u, v are such that

$$\mathrm{E}uv^T = I,$$

with I being the identity matrix, then it is easy to see that $H(x)$ is an unbiased estimator of the gradient of f at x. This simple observation proved to be amazingly useful if properly applied. The minimization of f can be carried out using H in a stochastic gradient method, thus yielding the SPSA method. This stochastic approximation scheme is similar to the well-known Kiefer-Wolfowitz scheme, but it is using just two measurements as opposed to $2p$ measurements, where p is the dimension. The clever choice of the vectors u and v is a key ingredient of SPSA.

We shall give a brief overview of the basic convergence results, including asymptotic covariance matrices, and rate of convergence for higher order moments. A few extensions of the original SPSA method will be also presented. In the second order SPSA method, also due to J. Spall, the Hessian matrix is estimated similarly to the gradient. The possibility of using higher order difference schemes to estimate the gradient will be also discussed.

A hybrid optimization approach for solving automated parameter-estimation problems. **Leticia Velazquez** (University of Texas at El Paso, USA), Hector Klie (University of Texas at Austin, USA), Mary Wheeler (University of Texas at Austin, USA), Miguel Argaez (University of Texas at El Paso, USA), Carlos Quintero (University of Texas at El Paso, USA) IC/MT4996/067

We present a hybrid optimization approach for solving automated parameter estimation problems that is based on the coupling of the Simultaneous Perturbation Stochastic Approximation and a globalized Newton–Krylov interior-point algorithm presented by Argáez *et al.* The procedure generates a surrogate model on which the interior-point algorithm can be used to find an optimal solution. We implement the hybrid optimization algorithm on several test cases, and present some encouraging numerical results.

Tuning machine-translation parameters with SPSA. **Rafael Banchs** (Universitat Politècnica de Catalunya, Spain), Patrik Lambert (Universitat Politècnica de Catalunya, Spain) IC/MT2176/067

Most of statistical machine translation systems are combinations of various models, and translation quality can be improved by adjusting the weight of each feature function in the log-linear combination. However, this optimisation problem in multiple dimensions is difficult because of three main characteristics of the objective function. Firstly, it has no analytic representation, so the gradient cannot be calculated. Secondly, it has many local minima. Finally, its evaluation has a significant computational cost.

Consequently, optimisations starting from different initial settings can converge to fairly different solutions. We present tuning experiments with the Simultaneous Perturbation Stochastic Approximation (SPSA) algorithm, and compare them to tuning with the widely used downhill simplex method. The objective of the experiment was to compare the consistency of the results over changes in initial settings. For this, we ran the algorithms from 7 different initial points and for each point, for 10 slightly different realisations.

With Chinese–English data from IWSLT 2006 machine translation evaluation, both methods showed similar performance, but SPSA was more robust to the choice of initial settings and with respect to slightly different realisations of the algorithm.

The conjugated effect of two SPSA properties not shared by the simplex method may contribute to explain this difference in stability. Firstly, SPSA search path follows in average the direction of the gradient, whereas the simplex orientation is blind. Secondly, SPSA has always a probability to go away from a zone close to a minimum, which allows it to find a lower minimum elsewhere in the search space. On the contrary, when the simplex shrinks in a zone close to a minimum, it is stuck in that zone.

SPSA for oil-parameter estimation and reservoir management. **Adolfo Rodriguez** (University of Texas at Austin, USA), Hector Klie (University of Texas at Austin, USA), Mary Wheeler (University of Texas at Austin, USA) IC/MT1498/067

The simultaneous perturbation stochastic approximation (SPSA) algorithm is emerging as a powerful but simple strategy for performing large-scale global optimization in several application settings. Two important features of this algorithm are: (1) it does not require derivative information; and, (2) the number of function evaluations is one or, at most two, independent of the size of the parameter space. In this work, we study the computational capabilities of SPSA under the view of two fundamental application from the oil industry: parameter estimation and, the optimal well placement. The parameter estimation problem (history matching) is a highly ill-posed and time-consuming task since the number of observations (on the order of hundreds to thousands) is relatively small compared to the number of parameters to be estimated (on the order of hundred of thousands to millions). To cope with this high complexity, we use SPSA in conjunction with a multiscale pa-

rameterization approach that allows us to dramatically reduce the parameter space. The estimation and sampling performed by SPSA is further enhanced by a neural learning engine that evaluates the objective function sensitivity with respect to parameter estimates in the vicinity of the most promising optimal solutions. The determination of the optimal well location is a challenging problem in oil reservoir management since it depends on both geological and fluid properties as well as on economic parameters. Traditionally, this task has been carried out by analyzing a few scenarios with a numerical reservoir simulator. This approach, however, has often led to misleading decisions with high economic impacts. SPSA offers the possibility of performing a systematic exploration of a broader set of well location and production scenarios with a lesser number of simulations. Numerical experiments show the viability of the method for addressing realistic problems.

IC/MP337/015: **Recent advances in large-scale optimization.**

Organiser: Michael Ulbrich (TU München, Germany)

Large scale optimization problems are of central importance in a wide range of applications. In particular, they arise whenever complex systems are involved in the optimization task, e.g., systems that are governed by PDEs, are coupled or networked, involve uncertainty, etc. Theory and methods for large scale optimization problems are the indispensable prerequisite for performing the crucial step from modelling and simulation to optimization and control of large systems. The aim of this minisymposium is to present important recent advances in selected fields of large scale optimization that are of general interest. The talks cover an attractive range of topics such as new algorithmic developments in large scale and infinite dimensional optimization, structure-exploiting algorithms, and challenging applications in engineering, geology, and finance.

Optimization problems in finance. **Ekkehard Sachs** (Universität Trier, Germany & Virginia Tech, USA), Kaebe Christoph (Universität Trier, Germany) IC/MT3567/015

The pricing of derivatives has gained considerable importance in the finance industry and leads to interesting problems in numerical optimization. We review some of the models for option prices and their practical application. The calibration of these models leads to optimization problem which can be large scale. We consider the numerical solution and show the efforts to reduce the complexity.

Inverse seismic wave propagation: algorithmic concepts and numerical results for real geological data. **Carsten Burstedde** (University of Texas at Austin, USA), Omar Ghattas (University of Texas at Austin, USA) IC/MT3204/015

The numerical solution of inverse problems in seismic wave propagation is a great challenge. The character of the waveforms in combination with a standard L_2 norm for the data misfit functional leads to highly nonlinear optimization problems with many local minima. A successful strategy here is to use multiscale hierarchies both in the space discretization and the signal frequencies. Alternatively, experience from computational seismology suggests to amend the data misfit term by observations of traveltime, phase shifts or more general integral transform operators. To improve the convergence of large-scale computations and accommodate different regularization approaches, we make use of limited-memory preconditioning and modifications of the Newton solver. We combine these ideas for the solution of inversion problems on real geological data and provide a variety of numerical results, and comment on the ongoing development of our massively parallel inversion code in three dimensions.

Aerodynamic shape optimization. **Volker Schulz** (Universität Trier, Germany) IC/MT1895/015

The efficient solution of aerodynamic shape optimization problems is of utmost importance for reducing fuel consumtion and/or improving aerodynamic characteristics of airplanes. This problems leads to large scale optimization problems, where the high number of variables corresponds mainly to the discretization of the PDE modeling the aerodynamic flow. One of the peculiarities of these problems lies in the fact that the flow solver to be used is mostly given from practicioners and represents a large volume of knowledge. That means that the flow solver can only be slightly changed and nevertheless an efficient optimization procedure should be constructed. Results and experiences from the German project MEGADESIGN will be presented.

Primal-dual interior-point methods for optimization problems with PDE constraints. **Michael Ulbrich** (TU München, Germany) IC/MT3237/015

Primal-dual interior-point methods have proven to be very efficient in the context of large scale nonlinear programming. In this talk, we present a convergence analysis of a primal-dual interior-point method for PDE-constrained optimization in an appropriate function space setting. Considered are optimal control problems with control constraints in L^p. The extension to state constraints is currently under investigation and we hope that we can present some progress also in this direction. It is shown that the developed primal-dual interior-point method converges globally and locally superlinearly. Not only the L^∞-setting is analyzed, but also a more involved L^q-analysis, $q < \infty$, is presented. In L^∞, the set of feasible controls contains interior points and the Fréchet differentiability of the perturbed optimality system can be shown. In the L^q-setting, which is highly relevant for PDE-constrained optimization, these nice properties are no longer available. Nevertheless, using refined techniques, a convergence analysis can be carried out. In particular, two-norm techniques and a smoothing step are required. Numerical results are presented that prove the efficiency of the method.

(Work done in collaboration with Stefan Ulbrich.)

06: Optimization, Contributed Talks

IC/CTS4658/06: **Optimal control, I.**

Organiser: Lino Alvarez-Vazquez (Universidad de Vigo, Spain)
Co-organiser: Aurea Martinez (Universidad de Vigo, Spain)

Optimal treatment planning in radiotherapy based on Boltzmann transport calculations. **Matthias Schaefer** (TU Kaiserslautern, Germany), Martin Frank (TU Kaiserslautern, Germany), Michael Herty (TU Kaiserslautern, Germany) IC/CT2114/061

A Boltzmann transport model for dose calculation in radiation therapy is considered. We formulate an optimal control problem for the desired dose. Based on this model we derive the optimality conditions for the full model as well as for approximate P_N models in 1d and 2d. We prove existence and uniqueness of the minimizer. We show that the P_N approximation of the optimality system is in fact the optimality system of the P_N approximation. Numerical results based on the P_N models in one and two dimensions are presented.

High-intensity ultrasound focusing by optimal acoustic lens design. **Slobodan Veljović** (Universität Erlangen–Nürnberg, Germany), Barbara Kaltenbacher (Universität Stuttgart, Germany) IC/CT1540/061

Shape optimization of an acoustic lens is considered. The problem comes from the usage of ultrasound in medical treatment of kidney stones. Since it can be assumed that no topology changes take place and only small geometry modifications have to be taken into account, we can work with gradient type optimization methods on a parameterization of the lens shape. For this purpose, the lens is parameterized by cubic splines and as a first step, the linear wave equation with jumping coefficients is used to represent wave propagation through the entire domain consisting of the fluid region (i.e., the human tissue) and the lens region. I.e. our model consists of the equation $\psi_{tt} - c^2\Delta\psi = 0$, where the speed of sound c is piecewise constant taking different values inside and outside of the lens. The cost functional is of tracking type to achieve an acoustic pressure distribution that exhibits a point focus at the desired location and has low amplitudes elsewhere. A sensitivity analysis is performed whose results are used in the numerical computations based on gradient methods using adjoint techniques for efficient gradient evaluation. Numerical results are presented and convergence issues as well as extension to a refined model consisting of a nonlinear wave equation in the fluid region and linear elasticity for the lens are discussed.

Optimal operation for a river fishway. **Lino Alvarez-Vazquez** (Universidad de Vigo, Spain), Aurea Martinez (Universidad de Vigo, Spain), Miguel Vazquez-Mendez (Universidade de Santiago de Compostela, Spain), Miguel Vilar (Universidade de Santiago de Compostela, Spain) IC/CT1164/061

A fishway (also known in the literature as fish ladder or fish pass) is a hydraulic structure that enable fish to overcome obstructions (dams, waterfalls, rapids...) to their spawning and other river migrations. We deal here with the more usual type of fishway: the vertical slot fishway. It consists of a rectangular channel with a sloping floor that is divided into a number of pools. Water runs downstream in this channel, through a series of vertical slots from one pool to the next one below. The water flow forms a jet at the slot, and the energy is dissipated by mixing in the pool. The fish ascends, using its burst speed, to get past the slot, then it rests in the pool till the next slot is tried.

We present a mathematical formulation of an optimal control problem related to a vertical slot fishway, where the state system is given by the shallow water equations determining the height of water and its velocity (averaged in height), the control is the normal flux of water on the inflow, and the objective function is related to the existence of rest areas for fish and a water velocity suitable for fish leaping and swimming capabilities: Our main aim consists of finding the optimal normal flux of incoming water for the vertical slot fishway so that the higher number of fish can ascend through the obstacle in the river in their best conditions.

We obtain a first order optimality condition for characterizing the optimal solutions of this problem, obtained by adjoint state techniques. From a numerical point of view, we use a characteristic-Galerkin method for solving the shallow water (Saint Venant) equations, and a derivative-free algorithm for the computation of the optimal control. Finally, we present numerical results obtained for the nine pools channel under study.

Optimal reclamation of polluted rivers. **Aurea Martinez** (Universidad de Vigo, Spain), Lino Alvarez-Vazquez (Universidad de Vigo, Spain), Miguel Vazquez-Mendez (Universidade de Santiago de Compostela, Spain), Miguel Vilar (Universidade de Santiago de Compostela, Spain) IC/CT1172/061

The main goal of this work is to use mathematical modelling and numerical optimization to obtain the optimal purification of a polluted section of a river. The most common technique for doing this consists of the injection of clear water from a reservoir in a near point. This strategy presents a high efficiency to purify polluted rivers in a short period of time. In this process of water injection the main problem consists, once the injection point is selected by geophysical reasons, of finding the minimum quantity of water which is needed to be injected into the river in order to purify it up to a fixed threshold. The goal of this paper is to determine this minimal quantity of injected water in order to ensure that the contaminant concentration in the river section is lower than fixed thresholds.

We formulate the problem as an optimal control problem, where the state system is given by the 1D shallow water equations coupled with the pollutant concentration equation, the control is the flux of injected water, and the objective function is related to the quantity of water and the pollution thresholds.

We present the mathematical formulation of the continuous problem, deriving a first order optimality condition in order to characterize the optimal solutions. We also analyse the discretization of the optimal control problem by means of a finite elements method, obtaining the discretized adjoint system and the gradient of the cost function. Finally, we deal with the numerical resolution of a realistic problem, where the optimization algorithm is introduced and computational results are provided.

Optimal control for supply-network models: adjoint calculus. **Claus Kirchner** (TU Kaiserslautern, Germany), Simone Göttlich (TU Kaiserslautern, Germany), Michael Herty (TU Kaiserslautern, Germany), Axel Klar (TU Kaiserslautern, Germany) IC/CT1914/061

We consider a PDE–based supply network model with controllable nodes for which we derive an optimal control problem and present an adjoint–based solution technique.

The supply network has two basic building blocks. The dynamics in a processor are governed by a PDE with a non-differentiable flux function. The behavior inside a queue is described by an ODE. The network model provides a framework to couple these equations at junctions. We introduce controls at certain junctions and discuss suitable cost–functionals leading to optimal control problems which we solve by a projected gradient method. The gradient information can be obtained from adjoint equations which we derived in the context of our supply network model. Finally we compare the numerical results, in particular the optimal controls, to a slightly different approach based on a mixed integer program.

Optimal control for supply-network models: mixed integer programming. **Simone Göttlich** (TU Kaiserslautern, Germany), Michael Herty (TU Kaiserslautern, Germany), Axel Klar (TU Kaiserslautern, Germany), Armin Fügenschuh (TU Darmstadt, Germany), Alexander Martin (TU Darmstadt, Germany) IC/CT2412/061

In this talk, we present a continuous model for the simulation and optimization of supply networks. We survey the underlying fundamentals, introduce a basic model based on partial and ordinary differential equations and show its relation to mixed-integer programming. This is done by applying numerical discretization schemes to the dynamics of the PDE and by approximations to the cost functional. The proposed MIP model is different from standard approaches due to its derivation from continuous dynamics. One benefit of the MIP model is the adaptivity to real-world situations by adding reasonable extensions such as bounded queues and the maintenance of processors.

IC/CTS4670/06: VIs, complementary equilibrium problems.

Organiser: Alexander Engau (Clemson University, USA)
Co-organiser: Vasile Preda (University of Bucharest, Romania)

Efficiency and optimization. **Vasile Postolica** (Bacau State University, Romania) IC/CT1252/006

This contributed talk is devoted to a new study concerning the main connections between efficiency and optimization. At the beginning, we present some important questions regarding efficiency and we emphasize the Pareto Optimality as one of the illustrative examples. Afterwards, following our recent concept of *approximate efficiency*, we indicate topical results obtained in infinite-dimensional spaces: strong links between efficiency, approximate efficiency, strong and vectorial optimization, potential theory and its applications through the agency of Choquet boundaries. To continue the scientific investigations, we include significant comments, pertinent remarks, adequate open problems and proper references.

Keywords: Efficiency, Approximate Efficiency, Pareto Optimality, Optimization, Potential Theory, Choquet Boundary.

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On a predictor–corrector method for a class of equilibrium problems. **Vasile Preda** (University of Bucharest, Romania), Miruna Beldiman (University of Bucharest, Romania), Anton Bătătorescu (University of Bucharest, Romania) IC/CT2878/064

We consider two classes of generalized monotone functions and generalized skew symmetric functions. By applying the auxiliary principle technique, we propose and study a predictor-corrector algorithm for solving mixed quasiequilibrium problems involving σ-pseudomonotone functions with respect to a ξ-skew symmetric bifunction. It is proved the convergence of the iterative sequence under generalized pseudomonotonicity and skew-symmetry assumptions, improving some known results in the recent literature.

On Tamir's algorithm for solving the nonlinear complementarity problem. **Uwe Schaefer** (Universität Karlsruhe, Germany) IC/CT1444/064

In 1974, Tamir published an algorithm for solving the nonlinear complementarity problem for the case that the given function is a so-called Z-function. This algorithm was a generalization of Chandrasekaran's algorithm which solves the linear complementarity problem for the case that the given matrix was a so-called Z-matrix. Proving his results Tamir used the iterative processes of Gauss-Seidel and Jacobi. We present a different proof where the iterative processes of Gauss-Seidel and Jacobi are not used.

On the regularity of dynamic equilibrium problems and computational procedure. **Annamaria Barbagallo** (Università degli Studi di Catania, Italy) IC/CT715/064

The aim of the talk is to consider dynamic equilibrium problems expressed by evolutionary variational and quasi-variational inequalities and to introduce a discretization method to calculate equilibrium solutions. The computational procedure is obtained after having shown the continuity of solutions to evolutionary variational and quasi-variational inequalities. In the detail, we obtain the continuity results for strongly monotone variational and quasi-variational inequalities, making use of concepts of the sets convergence in Mosco's sense and of Minty's Lemma. Then, we extend regularity results for strictly monotone evolutionary variational and quasi-variational inequalities using a regularity procedure. Finally, taking into account of the continuity, we present a discretization procedure and then we compute, by means of a projection-contraction method, solutions of the finite-dimensional variational inequalities obtained using the discretization. At last, we construct an approximation solution with the linear interpolation.

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Dimension reduction in multiobjective optimization. **Lino Costa** (Universidade do Minho, Portugal), Pedro Oliveira (Universidade do Minho, Portugal) IC/CT2246/067

In multiobjective optimization there is often the problem of the existence of a large number of objectives. For more than two objectives there is a difficulty with the representation and visualization of the solutions in the objective space. Therefore, it is not clear for the decision maker the trade-off between the different alternative solutions. Thus, this creates enormous difficulties when choosing a solution from the Pareto-optimal set and constitutes a central question in the process of decision

making. Based on statistical methods as Principle Component Analysis and Cluster Analysis, the problem of reduction of the number of objectives is addressed. Several test examples with different number of objectives have been studied in order to evaluate the process of decision making through these methods. Preliminary results indicate that this statistical approach can be a valuable tool on decision making in multiobjective optimization.

Multi-objective decomposition with applications in finance and engineering design. **Alexander Engau** (Clemson University, USA) IC/CT4282/067

Many optimization problems in finance, engineering, and numerous other fields require the simultaneous consideration of several criteria and, thus, are best modeled and solved using the methods from multiobjective programming and multicriteria optimization. A common characteristic of all these problems is that, in general, there does not exist a unique optimal solution, but a set of so-called Pareto solutions from among which the decision maker chooses based on personal preferences or additional criteria not included in the original optimization model. While a great variety of approaches exists to generate parts of the Pareto set, however, choosing a final preferred solution still remains difficult, especially if the numbers of objectives and solutions are too large to allow the effective use of an existing enumeration or visualization technique.

In remedy of these challenges and the generally high complexity encountered in real-life optimization problems, a multiobjective decomposition-coordination framework is proposed that initially decomposes the original objective function and forms a collection of smaller-sized subproblems that can be solved for their individual solution sets. To identify a common solution for all decomposed and, thus, the original problem, two subsequent coordination procedures are formulated that use the concept of epsilon-efficiency to integrate decisions on the desired tradeoffs between these individual solutions.

Two real-life applications are presented to illustrate the decomposition and the two coordination procedures for both a continuous and a discrete optimization problem. The first example is drawn from classical portfolio optimization and shows how the proposed approach enables the simultaneous consideration of several mean-variance estimators to arrive at a more reliable final investment portfolio. The second example describes a design selection problem in the context of automobile safety and shows how an initial set of simulated designs can be effectively reduced to only few efficient designs of particular interest to the designer and decision-maker.

IC/CTS4677/06: Queuing and probabilistic models.

Organiser: Ana Friedlander (Universidade Estadual de Campinas, Brazil)

On the $MX/G/1$ queueing system with first n exceptional services in each busy period. **Manju Sharma** (R B S College, Agra, India) IC/CT593/010

In this paper, we study a single-server queueing system in which customers arrive in groups of random size according to a time-homogeneous Poisson process and are served singly. The batches are served in order of their arrival, while the customers from the group are selected at random for service.The service time distribution depends on the number of customers served since the beginning of current busy period. However, it is assumed that the service time distribution becomes stable after N customers has been served in the current busy period. So, first N customers of each busy period receive exceptional services.

By using supplementary variable technique, recursion formulas are derived to obtain the generating functions of the stationary queue length distribution and the sojurn time distribution. These type of queuing systems are well applicable in many real-life situations including the modern computer and communication systems.

Cost analysis of dual machine interference model with general arrival distribution. **Sant Sharan** (Dr. RML Avadh University, Faizabad, India) IC/CT420/063

Previous authors made no attempt to discuss the cost analysis of the machine interference model with general arrival distribution $G/M/C/K/N$. In this paper, an attempt has been made to discuss the cost analysis of the same model. Upon constructing the cost function, a fast converging computer oriented N-R method has been used to solve the non-linear function, involving service rate and hyper geometric functions including other parameters in order to yield total optimal cost. Finally, an efficient evaluation of performance measure in the form of cost and the sensitivity analyses have also been presented.

Hierarchical multilevel optimization for reliability target allocation in probabilistic design of decomposed systems. **Michael Kokkolaras** (University of Michigan, Ann Arbor, USA) IC/CT2820/015

Design optimization of complex engineering systems can often be accomplished only by decomposition. The system is partitioned into subsystems, the subsystems are partitioned into components, the components into parts, and so on. The outcome of the decomposition process is a multilevel hierarchy of system-constituent elements.

In previous work, we developed analytical target cascading (ATC), a methodology for solving hierarchical multilevel optimal design problems. In ATC, system design targets are cascaded to subsystems and components using the model-based hierarchy. An optimization problem is formulated and solved for each design subproblem to minimize deviations from propagated targets. Solving the subproblems using appropriate coordination strategies yields overall system compatibility. We have also extended the deterministic ATC formulation to account for uncertainties. Uncertain design optimization variables and parameters are modeled as random variables, and all ATC optimization subproblems are reformulated as reliability-based design optimization (RBDO) problems.

In RBDO, reliability is defined as the statistical estimate of satisfying probabilistically formulated design constraints. Although reliability is nowadays considered to be a system design criterion of primary importance, its target value is prescribed more or less arbitrarily as opposed to being assigned optimally. The vast majority of RBDO methods require the specification of reliability targets for each of the probabilistic design constraints. In this work, we extend the probabilistic formulation of the analytical target cascading methodology to include reliability targets in the vector of cascaded quantities. In this manner, we achieve balanced optimality vs. reliability tradeoffs for each element of the decomposed system while satisfying the overall system reliability target.

ϵ-alternative solutions of the optimal-control problems. **Akbar H. Borzabadi** (Damghan University of Basic Sciences, Iran) IC/CT1135/006

In this paper we introduce ϵ-alternative solutions of the optimal control problems, which it seems that is useful for applications. Since in analytical discussion, extract of these solutions may be difficult, by a metamorphosis in the space of optimal control (OCP), we try to extract approximate ϵ-Alternative solutions for OCP's. Finally some numerical examples are given.

Theoretical aspects of an inexact restoration method for solving bilevel programming problems. **Ana Friedlander** (Universidade Estadual de Campinas, Brazil) IC/CT2809/063

We study theoretical properties of a method for bilevel programming problems. This method is based in the inexact restoration technique and showed a good performance on problems that fail to verify the sufficient conditions required in its convergence proof. Our goal is to fundament theoretically this behaviour.

An optimization method for locating epileptic sources: applications on realistic models of the head. **Maha Farah** (Université de Technologie Compiègne, France), Abdellatif El Badia (Université de Technologie Compiègne, France), Tuong Ha-Duong (Université de Technologie Compiègne, France) IC/CT2959/125

This paper addresses the identification of epileptic sources inside the brain knowing electromagnetic measurements on a part of the scalp. We consider the Maxwell equations on the quasi-static approach which are formulated as : $\nabla \times E = 0$, $\nabla \times B = \mu_0 (\sigma E + J^p)$ where E and B are the electric and magnetic fields, σ the conductivity and J^p the source term that we are seeking to estimate. The first equation gives $E = -\nabla V$, and from the second we have :

$$\nabla \cdot (\sigma \nabla V) = \nabla \cdot J^p$$

In this paper, we present a method to solve the EEG inverse problem, which consists to find J^p knowing σ and measurements of the electric potential V on a subset of the scalp. We assume that the head is made up of three disjoint coated domains (scalp, skull and brain), in each of which the conductivity is constant. Otherwise the geometry of these domains can be arbitrary. We consider a finite number of pointwise dipolar sources inside the brain. Assuming the number of dipoles is known, we have established an algorithm which allows us to identify their locations and moments. Our method consists in minimizing a cost function that involves the solutions computed from both the prescribed and measured data through their values inside the domain and not only on the boundary like the least square method. We have showed the robustness of the method and established the Gateaux derivative in order to use a gradient method to solve the corresponding optimization problem. Numerical experiments on realistic models with data known only on a part of the scalp have been performed. They show the robustness and the performance of our method.

IC/CTS4680/06: Miscellaneous, II.

Organiser: Raphael Hauser (University of Oxford, UK)

SDP approximability of relative robust QP. **Raphael Hauser** (University of Oxford, UK) IC/CT3575/067

Consider the framework in which a utility function depends on a vector of uncertain parameters which are only known to lie in a given uncertainty set. Relative robust optimisation is a framework in which the objective function is defined as the loss of utility relative to a benchmark that would choose the optimising values for the decision variables if the uncertain parameter was known. Given this so-called regret function, one seeks to minimise (over the decision variables) the pessimised (over the parameter values in the uncertainty set) regret. The resulting problem is a tri-level optimisation problem which can be approximated by a tractable conic programming problem. We investigate this approximability and identify cases in which the tractable approximation solves the original problem. The resulting technique leads to interesting applications in robust portfolio optimisation, in a setting where the performance is measured relative to a benchmark.

First-order methods for semidefinite optimization and applications. **Alexandre d'Aspremont** (Princeton University, USA) IC/CT1342/063

We present some recent results on first order methods in semidefinite optimization and discuss applications in machine learning and statistics.

Interior-point methods specialized to optimal pump-operation costs of water-distribution networks. **Aurelio Oliveira** (Universidade Estadual de Campinas, Brazil), Aline Lima (Universidade Estadual de Campinas, Brazil) IC/CT2901/063

The water supply problem aims to deliver water from reservoirs to consumer points through a network flow system. Pumps are used in order to comply with water demand and network constraints. This problem can be formulated as a network flow model using Kirchhoff's laws with additional constraints to achieve minimal pressure in the nodes and bounds on arcs. This methodology intends to minimize pumping energy costs of water distribution networks. For this purpose a specialized interior point method is developed for this system in the same fashion as it is performed for electrical power transmission systems. The resulting formulation is nonlinear. It is approached as a quadratic objective function problem subject to generalized graph with additional constraints in an iterative way generating, thus, a sequence of quadratic problems. The resulting matrix structure that arises from the interior point methods is exploited leading to smaller linear systems to compute the search directions. Computational experiments are presented, showing the robustness and speed of this approach.

A continuous Newton-type method for unconstrained optimization. **Li-Zhi Liao** (Hong Kong Baptist University) IC/CT1328/010

In this talk, we will propose a continuous Newton-type method in the form of an ordinary differential equation by combining the negative gradient and Newton's direction. It is shown that for a general function $f(x)$, our method converges globally to a connected subset of the stationary points of $f(x)$ under some mild conditions; and converges globally to a single stationary point for a real analytic function. The method reduces to the exact Newton method if the Hessian matrix of $f(x)$ is positive definite. The convergence of the new method on 18 standard test problems in the literature are also reported.

Nash-equilibrium conditions for strategic form games. **Valeriu Ungureanu** (State University of Moldova) IC/CT605/064

The notions of the Lagrange vector-function and the saddle point are introduced for normal-form strategic games. The Nash equilibrium conditions are formulated and proved. The Pareto–Nash equilibrium conditions are formulated for multi-criteria strategic form games. Other different Pareto-Nash, weak Pareto–Nash (Slater–Nash) etc. equilibrium conditions may be formulated and proved for multi-criteria games. Well-known theorems for matrix games are extended on strategic form games. Mathematical programming Kuhn–Tucker theorems are extended on strategic form games. Well-known theorems for multi-criteria optimization problems are extended on multi-criteria strategic form games. The theoretical and practical impacts of the obtained results are analyzed.

Elastic–plastic deforming of a heterogeneous media. **Victor Yanko** (Dnipropetrovs'k National University, Ukraine) IC/CT1390/006

A theoretical model which allows to define the effective elastic–plastic properties of a heterogeneous multiphase material is proposed here. It is supposed that elastic-plastic properties and the parameters describing spatial distribution of particles of each phase are known.

Firstly, some kinematical relations are derived. They include the laws of evolution of the phase relative volume as well as the symmetric second order tensor (phase tensor) which describes spatial distribution of the particles of each phase in the representative volume of the heterogeneous material. Also the relation between overall (effective) strain rate and strain rate of the phases is obtained from the condition of compatibility of deforming of all phases.

Then, with using of the equivalent inclusion method the procedure of localization is carried out. It allows to find the relations between local (phase) and effective deformation rates which includes fourth and second order strain concentration tensors. The first from them takes into account the heterogeneity of the tangent modulus, while the second tensor depends only from plastic components of local and effective strain rates and takes into account the heterogeneity of the plastic strain rate inside the material.

Finally, the procedure of homogenization is proposed. It based on condition of equality of the Cauchy stress vector which acts in the heterogeneous body and the sum of the phase stress vectors; each of them is applied to a particular phase. The resulting relation is divided to the "elastic" and "plastic" parts, what allows to find elastic L_e^H and plastic L_p^H components of the effective secant module $L_t^H = L_e^H - L_p^H$.

IC/CTS4664/06: Shape optimization.

Organiser: Mircea Lupu (Transilvania University of Brasov, Romania)
Co-organiser: Adriana Nastase (RWTH Aachen, Germany)

A level-set method for topology optimization using topological derivatives. **Samuel Amstutz** (Université d'Avignon, France), Heiko Andrä (Fraunhofer ITWM, Kaiserslautern, Germany) IC/CT2161/061

The level-set method has been recently introduced in the field of shape optimization, enabling a smooth representation of the boundaries on a fixed mesh and therefore leading to fast numerical algorithms. However, most of these algorithms use a Hamilton-Jacobi equation to connect the evolution of the level-set function with the deformation of the contours, and consequently they can hardly create new holes in the domain (at least in 2D). We propose an evolution equation for the level-set function based on a generalization of the concept of topological derivative. This results in a new algorithm allowing for all kinds of topology changes. In the talk, the method will be presented together with some numerical examples in structural optimization.

A shape optimization problem with convex constraint. **Arian Novruzi** (Université d'Ottawa, Canada) IC/CT4551/061

We consider the optimization of a shape functional over a set of 2D convex domains. This problem has been considered by M. Crouzeix, see [1], who by using surprising geometric elementary considerations proves that the solution is a polygon.

The problem represents a typical model of a larger class of problems and we consider it from a Hilbertian functional viewpoint. We find the Euler–Lagrange equation, see [2], which due to constrains invloves Radon measures. Contrary to shape optimization problems without constraint, or with equality constraints, here the Euler–Lagrange equation does not provide sufficient information to identify the solution. Using the second order necessary condition, see [3], we first characterize the solution up to a zero-measure set. Next, detailed analysis using again the second-order necessary condition leads to a complete charcterization of the regularity of the solution.

Work done in collaboration with Jimmy Lamboley and Michel Pierre, ENS Cachan, Antenne de Bretagne.

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[3] Maurer H., Zowe J.; First and second order necessary and sufficient optimality conditions for infinite-dimensional programming problems, Mathematical Programming 16, 1979.
[4] Simon J.; Differentation with respect to the domain in boundary value problems, Numer. Funct. Anal. and Optimiz., 2(7), pp.649–687 (1980).

Mixed integer programming for topology optimization in sheet-metal design. **Armin Fügenschuh** (TU Darmstadt, Germany), Alexander Martin (TU Darmstadt, Germany) IC/CT4199/066

Topology optimization lies at the heart of many design tasks in mechanical engineering. For those sheet metal products that consists of a bundle of separate channels (such as conduits) we formulate the design task as a linear mixed-integer optimization problem. The design goal is to find a topology where each channel has a given cross-section area, using a minimum amount of sheet metal. In addition to a light-weight design, stiffness should also be taken into account. The entire approach is demonstrated in the design of a conduit with several separate channels.

Surrogate modeling for geometry optimization in material design. **Marielba Rojas** (Danmarks Tekniske Universitet, Denmark) IC/CT1986/015

One of the main problems in material design is the determination of the electronic structure of a given material. The first step in electronic-structure calculations is geometry optimization, i.e. finding a stable arrangement of the atoms in a molecule.

One of the most popular and successful approaches for the study of materials is density-functional theory. Under this model, the calculation of the optimal geometry involves the

minimization of the total-energy functional. The evaluation of this functional for a given geometry is a time-consuming process.

Due to the cost of evaluating the objective function, the use of standard minimization techniques is prohibitive in practice. An alternative is the Car-Parrinello method, also called indirect optimization or quantum-molecular-dynamics approach, which avoids the direct evaluation of the total-energy functional. This method can be very expensive for large molecules and is not robust in general, especially for metals.

We have recently proposed a new approach for geometry optimization based on surrogate modeling. We use both splines and kriging to construct the surrogates. We describe our approach and present preliminary results on test problems and on a diamond crystal.

Joint work with Yonas B. Abraham, Computer Science, Natalie A.W. Holzwarth, Physics, and Robert J. Plemmons, Mathematics, Wake Forest University, Winston-Salem, North Carolina, USA.

Analytical-numerical methods in the curvilinear airfoils optimization of maximal or minimal drag in hydro-aerodynamics. **Mircea Lupu** (Transilvania University of Brasov, Romania) IC/CT3839/061

In this paper are solved direct and inverse boundary value problems and is obtained analytical and numerical the solution for the problem optimization, in the case of nonlinear integral operators. We considered the plane potential flow of an inviscid, incompressible and limited or unlimited fluid jet, which encounters symmetrical curvilinear obstacle; it is modeled the design in the case maximal or minimal drag. There are derived for direct and inverse problems the singular integral equations and it is obtained the movement in the auxiliary canonical half plane. Using my results of the integral equations method we obtained the analytical solution, considering a general distribution of the speed on the profile. The nonlinear operators of the drag are maximized using a Jensen type inequality. The drag coefficient and other parameters geometrical and aerodynamical are computed numerically in the special general case of Helmholtz or Rethi - Bobilev - Jacob scheme. We restart by the Newton Problem, in the case of the minimal drag problems for the same scheme and thought the inverse method it is given apriority the speed on profile in the singular equations it is determined the drag resultant minimal. We apply penalty method and we determined the profile design. These results are applied trust reversal devices, to the control of the direction of area reactive vehicle, to the design of the wings of an airplane, of the blades of a turbine or of the bracket parachute.

An iterative optimum-optimorum theory for global optimal shape design. **Adriana Nastase** (RWTH Aachen, Germany) IC/CT1989/067

IC/CTS4679/06: Miscellaneous, I.

Organiser: Enrico Miglierina (Università dell'Insubria, Italy)

Iterated hard shrinkage for linear inverse problems with sparsity constraints. **Dirk Lorenz** (Center for Industrial Mathematics - University of, Germany), Kristian Bredies (Universität Bremen, Germany) IC/CT1838/065

In this talk we describe an iterative algorithm for the minimization of Tikhonov type functionals which involve sparsity constraints in form of ℓ^p-penalties which have been proposed recently for the regularization of ill posed problems.

In contrast to the well-known algorithm considered by Daubechies, Defrise and De Mol, it uses hard instead of soft thresholding. This hard thresholding algorithm is based on the generalized conditional gradient method. General results on the convergence of the generalized conditional gradient method enable us to prove strong convergence of the iterates. Furthermore we are able to establish convergence rates of $\mathcal{O}(n^{-1/2})$ and $\mathcal{O}(\lambda^n)$ for $p = 1$ and $1 < p \leq 2$ respectively.

Numerical experiments on image deblurring and backwards heat condution are given and illustrate the established convergence rates.

Fuzzy linear-programming model for optimal farmlands fertilization. **Edmundo Vergara** (Universidad Nacional de Trujillo, Peru) IC/CT856/010

The use of the fuzzy logicŠs theoretic concepts has permitted in this work to make the mathematical model on fertilization in farming land, as a model of fuzzy linear programming whit fuzzy equality constrained, said the fuzzy diet model for fertilization in farming land. This model has solved using three methods, VerdegayŠs method, ZimmermannŠs method and WernersŠs method format.

Ecological management problem with changing protected area for fishery. **Vladimir Mazalov** (Karelian Research Centre of the RAS, Russian Federation) IC/CT3464/064

A dynamic game model of bioresource management problem is considered. There are two players: the center which determines a share of protected area of the lake where fishery is prohibited and the fishing farm which is harvesting in non-protected area. In traditional statement the center's strategy is the catch regulation by introduction quotas on fishing. We propose the approach where the center's strategy is the choice of optimal share of protected area for maintenance of stable population developement in the lake. We consider finite and infinite planning horizon and use the maximum principle and Hamilton-Jacobi-Bellman equation to derive the Nash equilibrium in the game.

The dual diagnosis of an aircraft command. **Octavian Grigore-Müler** (Universitatea Tehnicã Bucarest, Romania) IC/CT2716/068

As part of a programme investigating the design of new aircraft which are intended to be much more efficient and reliable in their use that those currently in service, the aeronautics and automatics engineers are studying aircraft and systems which would operate with greatly reduced stability margins and would as a result be totally dependent on computer control for the safety of a flight. So these computer systems generally used to provide active control should be required to have efficient diagnosis systems. A fuzzy dual diagnosis system for a command of a commercial airplane is presented.

Well-posedness and stability for abstract spline problems. **Enrico Miglierina** (Università dell'Insubria, Italy), Elena Molho (Università di Pavia, Italy) IC/CT4017/063

Spline functions play a fundamental role in many fields of numerical analysis and statistics and they are involved in many important applications, for instance in engineering, economics, biology and medicine.

The variational approach to interpolation techniques has been fruitfully employed to obtain existence and uniqueness results for interpolating spline functions. An abstract unifying framework for this topic is classically developed in the setting of Hilbert spaces. Here, following a more general approach, we consider the problem in the setting of reflexive spaces. The aim of this work is to study well-posedness and stability properties of the abstract spline problem.

The property of well-posedness of an optimization problem essentially requires that the minimizing sequences are well-behaved. This is a relevant feature in order to individuate those problems that can be studied through direct methods and to develop efficient numerical procedures. Here, we show that the same assumptions that usually ensure existence and uniqueness of a solution for an abstract spline problem also imply the stronger property of well-posedness.

The study of the stability properties of some special parametric families of abstract spline problems has already been developed in the literature. Here we consider sequence of parametric problems converging to the given abstract spline problem in order to study stability properties. Under natural assumptions, we obtain new some convergence results for sequences of solutions of the perturbed problems in the case of general version of the abstract spline problem. These results are refined in the special case where the admissible region is an affine set and, in particular, it is determined by a set of evaluation functionals, as in the classical interpolation problem.

Optimal operation mode for distributed cogeneration power plants. **Nadia Maïzi** (Ecole des Mines de Paris, France), Marc Bordier (École des Mines de Paris, France) IC/CT3348/015

Cogeneration systems combine electrical (or mechanical) and useful thermal energy from the same primary energy source. As the efficiency increases from 0.58 for a separate production of electricity and heat, to 0.85 for the cogeneration, they allow a considerable decrease in total fuel consumption. But beside these environmental issues, the economical viability of the cogeneration project remains the main issue for operators. It relies on many factors, among which the mode of operation of the cogeneration system. In this study, we will focus on the heat-match mode where the priority is to satisfy a heat demand. The amount of excess electricity is exported to the grid, while the lack of electricty is bought from an electricity market.

In the framework of the heat-match mode operation, we consider an operator who operates over a given designed (type of the technology, size, configuration) set of cogeneration units. The purpose of this paper is to determine the best operating mode in order to minimise the cost of operation of the whole cogeneration system. The optimisation procedure is achieved through two steps:

1. we consider a single unit and develop an explicit formulation of the optimal mode of operation, when the operator knows the heat and power demand, and the electricity price on the market;
2. we express for the overall cogeneration system the operating cost: the objective function is still convex but non differentiable. Thus, it requires an optimisation procedure based on subdifferential calculus: through namely the Moreau–Rockafellar and Duboviskii–Milyutin theorems.

Then, the result describing the best operating mode for the overall set of cogeneration units relies on the value of the marginal costs associated with each mode of operation, for each unit: optimal operation of the cogeneration power plant is achieved through an economic dispatch mode.

IC/CTS4682/06: Inverse problems: identification.

Level-set and adjoint-based optimization methods for inverse problems. **Frédéric Chantalat** (Université Bordeaux I, France), Charles-Henri Bruneau (Université de Bordeaux, France), Angelo Iollo (Université de Bordeaux, France) IC/CT2359/065

As a preamble for drag-reducing studies on Stokes flows, inverse obstacle problems governed by Laplace and Poisson equations have been considered. Dirichlet boundary conditions have been applied on both the top/bottom edges of the computational domain and the geometry interface, whereas Neumann boundary conditions have been used on the remaining edges. Shape optimization is handled by finite differences discretization of the continuous adjoint equations on a cartesian mesh. A level-set function ϕ defined below, sign-changing across the interface, enables the localization of the body by providing the distance of each node from its border.

$$\begin{cases} \phi(x,y) < 0 \;\; if \;\; (x,y) \in \Omega_{obstacle} \\ phi(x,y) > 0 \;\; if \;\; (x,y) \in \Omega - \Omega_{obstacle} \\ phi(x,y) = 0 \;\; if \;\; (x,y) \in \partial\Omega_{obstacle} \end{cases}$$

At each step, after determination of the shape-derivative, and alteration of the boundary, Fast-Marching methods operate a redistanciation process. Both direct and adjoint equations are solved by the GMRES algorithm thanks to a penalization method. However, an iterative procedure aiming at finding a consistent extension of the solution inside the penalized zone is added so that the gradient evaluation along the normal $\frac{\nabla\phi}{|\nabla\phi|}$, often inaccurate due to the use of this type of mesh can be significantly improved. Even though Level-Set methods prove to be quite efficient in terms of dealing with topoligical changes, such inverse problems appear to be severely ill-posed, causing gradient-based methods to fall into local minima regions. Thus, a study of the choice of the objective function has been carried out showing the relevance of a multiscale approach where large, medium, and small contributions follow one another along iterations in W-shaped cycles. Another way to make the problem more sensitive to shape variations was inspired by scanning techniques used in medical imagery. The angle from which the obstacle is observed is modified by rotating the obstacle during the optimization algorithm thanks to a fifth-order WENO scheme for transport equation. This method also has a drastic influence on speeding up convergence. The presentation emphisizes the role of such numerical tools in the previous cases along with an extension of the work on inverse Stokes' problem.

Newton methods for nonlinear inverse problems with random noise. **Frank Bauer** (Universität Linz, Austria), Thorsten Hohage (Universität Göttingen, Germany), Axel Munk (Universität Göttingen, Germany) IC/CT1038/065

The solution of nonlinear operator equations $F(a) = u$ by iterative regularization methods with deterministic noise has been studied intensively over the last decade. However, we are not aware of any convergence and convergence rate results of iterative regularization methods for nonlinear inverse problems with random noise. Moreover well-known stopping rules like Morozov's discrepancy principle do not work in this situation.

We will present a slightly modified iteratively regularized Gauss-Newton method with the Lepskij-type balancing principle as a-posteriori stopping rule.

We do not need any restrictive assumptions on the structure or the degree of nonlinearity of the operator F, but only have to require Lipschitz continuity of F' and a sufficiently strong source condition. As a result we obtain almost optimal rates of convergence over a range of Hölder smoothness classes.

Shape methods for the transmission problem with a single measurement. **Lekbir Afraites** (UTC Compiegne france) IC/CT703/061

In the present work, we consider the inverse conductivity problem of recovering inclusion with one measurement. First, we use conformal mapping techniques for determining the location of the anomaly and estimating its size. We then get a good initial guess for quasi-Newton type method and Newton method. The inverse problem is treated from the shape optimization point of view. We give a rigorous proof for the existence of the first and second order shape derivative of the state function and of shape functionals. We consider both Least Squares fitting and Kohn and Vogelius functionals. For the numerical implementation, we use a parametrization of shapes coupled with a boundary element method. We compare the results obtained by quasi-Newton and Newton. Several numerical exemples indicate the superiority of the Kohn and Vogelius functional over Least Squares fitting.

This is a joint work with Dr. Djalil Kateb.

Heat-source and boundary-condition identifications of a 2D composite material with different thermal diffusivities in multi-block grids. **Aziz Azimi** (Sharif University of Technology, Iran), Siamak Kazemzadeh Hannani (Sharif University of Technology, Iran) IC/CT895/065

Inverse Heat Conduction Problems (IHCPs) frequently require the reconstruction of the unknown heat sources and boundary conditions using the measured temperature history of the sensors located at interior domain or near to boundaries. Solution procedure of these problems consists of three parts: 1. a numerical solution of Partial Differential Equations (PDEs), 2. a definition of error and minimization or optimization of it, 3. a regularization scheme to stabilize the usually ill-conditioned discretized system obtained in the second part. The regularization of the optimization procedure is required to avoid the extreme sensitivity of the solution of this procedure to the errors in the measured data. Iterative regularization scheme is one of the most efficient and universal approaches for solution of IHCPs.

In this research, iterative regularization algorithms based on two parameter estimation techniques are developed to solve two-dimensional transient IHCPs. Those of the PDEs needed for inverse analysis are used in their strong conservation forms to resolve discontinuities such as thermal conductivity and diffusivity at the material interfaces. A structured discretization of the computational domain of each block is done using a simple algebraic grid generation method. The computational code developed for numerical solution of the PDEs considers a central Finite Difference Method (FDM) in conjunction with the block-structured grids with interface blocked/ overlapped points. An Alternative Direction Implicit (ADI) technique is used for temporal discretizations of the PDEs in Cartesian coordinates system. The parameter estimation techniques used for inverse analysis are Levenberg-Marquardt and adjoint conjugate gradient methods. The temperature histories needed for parameter estimation are delivered by noisy/non-noisy sensors located on the upper or right boundary of the domain. Two cases are considered to show the ability of the developed code, a simultaneous estimation of two time-varying heat sources and an estimation of upper time-space varying boundary condition in surfaces with different thermal diffusivities. The results of the present study are compared to those of exact heat source and temperature boundary condition.

IC/CTS4674/06: Proximal and penalty methods.

Organiser: Alexander Zaslavski (Technion – Israel Institute of Technology)
Co-organiser: Igor Griva (George Mason University, USA)

Strong convergence of approximate proximal methods. **Lu-Chuan Ceng** (Shanghai Normal University, PR China) IC/CT4018/064

The purpose of this paper is to investigate approximate proximal algorithm and Bregman-function-based approximate proximal algorithm for solving the generalized variational inequality problem (for short, GVI(T,Ω) where T is a pseudomonotone multivalued operator). The goal for the present work is twofold. First, consider subproblems on the domains $\Omega_n \supset \Omega$, $n = 1,2,...$, which form a general approximate proximal point scheme. It is shown that this general approximate proximal point scheme generates a sequence, which converges strongly to a solution of GVI(T,Ω). Second, by virtue of a suitable Bregman function, define new approximating problems on the domains $\Omega_n \supset \Omega$, $n = 1,2,...$, which form a general Bregman-function-based approximate proximal point scheme for solving GVI(T,Ω). It is also proven that this general Bregman-function-based approximate proximal point scheme generates a sequence, which converges strongly to a solution of GVI(T,Ω).

On portfolio optimization using fuzzy decisions. **Sudradjat Supian** (Bucharest University, Romania), Vasile Preda (University of Bucharest, Romania) IC/CT3511/010

We consider stochastic optimization problems involving stochastic dominance constraints. We develop portfolio optimization model involving stochastic dominance constrains using fuzzy decisions and we concentrate on fuzzy linear programming problems with only fuzzy technological coefficients, aplication of modified subgradient method to fuzy linear programming problems.

Key words. stochastic programming, stochastic dominance, portfolio, fuzzy linear programming, optimality conditions, duality,. AMS subject classifications. Primary, 90B28, 90C15, 90C46, 90C70; Secondary, 46N10, 90B10, 91B06

Some characteristics of an investment project's efficiency. **Efim Bronshtein** (Ufa State Aviation Technical University, Russian Federation) IC/CT505/015

The investment project is a vector $C = (c_0, c_1, \check{E}, c_n)$ of arbitrary finite dimension such that its first nonzero component is negative, $c_n > 0$, $\sum c_i > 0$. Negative components mean investments to the project at the corresponding time moments (years), positive - receipts to the investor. A few characteristics are usually applied for the comparative analysis of investment projects.

One characteristic of the investment project was defined by K.Arrow and D.Levhari [1]. Let $P_k(k = 1,2,...,n)$ be the functions of profitability of the truncated investment projects, i.e.$P_k(x) = \sum_{i=0}^{k} c_i x^{-i}$, where x is a year accumulation coefficient and $\psi(x) = max_k\{P_k(x)\}$.

PROPOSITION 1. The equation $\psi(x) = 0$ has a unique root $AL(C)$ in the set $[1,\infty)$.

The class of investment projects (named correct projects) and its efficiency characteristic (named limited profitability) were defined in [2]. Let us reminde here these definitions. Transaction is the year loan $(0,...,0,-a,b,0,...)$ where $b \geq a > 0$. The investment project is correct if it can be represented as the sum of some consecutive transaction. Correctness of the project is equivalent to the validity of the following conditions: $c_0 < 0$, $\sum_{i=k}^{n} c_i \geq 0$ for $k = 0,1,...,n$. The correct project can

be differently represented as the sum of transaction.

We define a profitability of the transaction as the relation b/a. A profitability of the sum of transactions is defined as a maximal of component's profitabilities. The limited profitability $LP(C)$ of the correct project is equal to the minimal profitability of the sums of the transaction representing project C.

PROPOSITION 2. $AL(C) = LP(C)$ for the correct investment projects.

Some properties of limited profitability showing its practical advantage are established in [2].

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Higher-moment risk measures: application to portfolio optimization. **Pavlo Krokhmal** (University of Iowa, USA) IC/CT3529/063

In this talk we discuss modeling of risk-averse preferences in stochastic optimization problems using risk measures. In particular, we consider the axiomatically defined risk measures, such as coherent risk measures (Artzner et al, 1999), deviation measures (Rockafellar et al, 2004), etc. We utilize the axiomatic foundation of coherent risk measures and deviation measures in order to develop simple representations that express risk measures via solutions of specially constructed (convex) stochastic optimization problems, which, in turn, can be seamlessly incorporated into the objective and/or constraints of mathematical programming models. As a special case of the developed general representations, we introduce a new family of higher-moment coherent risk measures (HMCR) that quantify risk via higher tail moments of loss distributions. It is shown that the family of HMCR measures can be implemented in mathematical programming problems using p-order cone programming. To facilitate incorporation of HMCR measures into existing decision-making models (such as portfolio optimization models, etc.), polyhedral approximations of p-order conic constraints are presented. Further, it is demonstrated that the HMCR measures are compatible with second order stochastic dominance and utility theory, in the sense that minimization of risk using an HMCR measure yields a SSD-efficient solution. A portfolio optimization case study illustrates the practical merits of employing the HMCR measures in an aggressive trading setting.

On existence of exact penalty in constrained optimization . **Alexander Zaslavski** (Technion – Israel Institute of Technology) IC/CT1431/063

In this talk we discuss the penalty approach in optimization and a very simple sufficient condition for the exact penalty property.

Support-vector machine via nonlinear rescaling. **Igor Griva** (George Mason University, USA), Shen-Shyang Ho (George Mason University, USA), Roman Polyak (George Mason University, USA) IC/CT1946/063

This talk presents a support vector machine (SVM) based on the nonlinear rescaling (NR) methodology. The formulation of the linear SVM based on the NR method leads to an algorithm that reduces the number of support vectors without compromising classification performance compared to the linear soft-margin SVM formulation. The dual variables provide important information about each data point and play the key role in selecting the set of support vectors. Experimental results on ten benchmark classification problems demonstrate that the quality of discrimination of the NR-SVM is comparable to the linear soft-margin SVM while the number of support vectors is substantially reduced.

IC/CTS4657/06: PDE control.

Organiser: Andrzej Myslinski (Polish Academy of Sciences, Poland)

Application of LQR techniques to the adaptive control of quasilinear parabolic PDEs. **Jens Saak** (TU Chemnitz, Germany), Peter Benner (TU Chemnitz, Germany) IC/CT2481/061

LQR problems for linear parabolic PDEs have been studied in detail in the literature for the past 3 to 4 decades. The solvability of feedback control problems for a large class of problems is well understood. In the recent years numerical methods for the approximation of the corresponding Riccati operators have been developed. These methods are able to calculate the feedback operator directly and thus can compute the solutions to linear problems efficiently.

Here we study the applicability of such techniques to the control of quasilinear equations via local linearization in an adaptive control setting.

Shape and topology optimization of contact problems by level-set method. **Andrzej Myslinski** (Polish Academy of Sciences, Poland) IC/CT3088/061

This paper deals with the formulation of a necessary optimality condition and numerical solution of the topology and shape optimization problems of an elastic body in unilateral contact with a rigid foundation. The contact with a given friction, described by Coulomb law, is assumed to occur at a portion of the boundary of the body. This contact problem is described by an elliptic inequality of the second order governing a displacement field. The optimization problem consists in finding, in a contact region, such shape of the boundary of the domain occupied by the body that the normal contact stress is minimized.

Level set methods are numerically efficient and robust procedures for the tracking of interfaces, which allows domain boundary shape changes in the course of iteration. The evolution of the level set function is governed by the Hamilton – Jacobi equation. The speed vector field driving the propagation of the level set function is given by the Eulerian derivative of an appropriately defined cost functional with respect to the free boundary.

In this paper the necessary optimality condition is formulated. The holes are supposed to be filled by weak phase mimicking voids. The level set method, based on the classical shape gradient, is coupled with the bubble or topological derivative method, which is precisely designed for introducing new holes in the optimization process. Since both methods capture a shape on a fixed Eulerian mesh and rely on a notion of gradient computed through an adjoint analysis, the coupling of these two method yields an efficient algorithm. Moreover the finite element method is used as the discretization method. Numerical examples are provided and discussed.

Boundary-optimal flow control with state constraints. **Juan Carlos de los Reyes** (Escuela Politécnica Nacional, Ecuador) IC/CT858/061

The boundary optimal control problem of the Navier–Stokes in presence of pointwise state constraints is studied. After discussing the choice of adequate control spaces, a Lavrentiev regularization of the problem is introduced. The regularity of the multipliers is studied and convergence of the regularized solutions towards the original one is proved. A semi-smooth Newton method is applied for the numerical solution of each regularized problem and numerical experiments are carried out.

Numerical solution of differential Riccati equations arising in optimal control for parabolic PDEs. **Hermann Mena** (Escuela Politécnica Nacional, Ecuador), Peter Benner (TU Chemnitz, Germany) IC/CT2517/061

The numerical treatment of linear-quadratic regulator problems on finite-time horizons for parabolic partial differential equations requires the solution of large scale differential Riccati equations (DREs). Typically the coefficient matrices of the resulting DRE have a given structure (e.g. sparse, symmetric or low rank). Here we derive numerical methods for solving DREs capable of exploiting this structure, which are based on a matrix-valued implementation of the BDF methods. The crucial question of suitable stepsize and order selection strategies will also be addressed.

Path-following methods in function space for state-constrained optimal control. **Anton Schiela** (Zuse-Institut Berlin, Germany) IC/CT1905/006

Pathfollowing methods in function space are widely considered as a very promising concept for the solution of optimization problems subject to PDE constraints and bounds on the state.

There are a number of different approaches available (e.g. barrier methods, penalty methods, Lavrentiev regularization), which all share the idea of solving a sequence of regularized problems by (semi-smooth) Newton methods in order to compute successive approximations of the desired solution.

Subject of this talk are theoretical results and algorithmic ideas that contribute to the understanding and implementation of this class of methods.

IC/CTS4661/06: Optimal control, II.

Organiser: Martin Fuchs (Universität Wien, Austria)
Co-organiser: Natalia Dmitruk (National Academy of Sciences, Belarus)

Uncertainty modeling in autonomous robust spacecraft design. **Martin Fuchs** (Universität Wien, Austria), Arnold Neumaier (Universität Wien, Austria), Daniela Girimonte (European Space Agency, The Netherlands) IC/CT4747/006

In the last years, much research has been dedicated to the achievement of decisions support systems to the space system engineers or even of autonomous design methods which try to capture the reasoning of the system experts. However, the problem of taking into account the uncertainties of the variables and models towards an optimal and robust spacecraft design has not been tackled effectively yet.

Traditional modeling of uncertainties faces several problems. In current methods considering worst case analysis the ignorance of distributions of uncertain variables or the ignorance of correlations between uncertain data, respectively, sometimes leads to underestimations of error probabilities. Moreover, even provided the knowledge of the multivariate probability distributions, in higher dimensions the numerical computation of the error probabilities is very expensive, if not impossible.

The new concept of **Clouds** for handling uncertainties was introduced by Neumaier, A. in 2004. Clouds are combining the concept of a fuzzy set and that of a probability distribution. They capture useful properties of the probabilistic and fuzzy uncertainties, enabling the user to utilize the collected empirical information (even if very limited in amount) in a reliable, validated way.

For given confidence levels the clouds provide regions of relevant scenarios affecting the worst case for a given design. In robust design, a design is considered unsafe if one of the relevant scenarios does not satisfy the safety-requirements. The concept, applied to the problem of optimization of robust spacecraft system design, aims at finding the optimal design with regard to the safety constraints and to the uncertainty information provided by expert designers.

On-line state estimation for nonlinear dynamical systems. **Natalia Dmitruk** (National Academy of Sciences, Belarus) IC/CT731/062

For a wide range of real-life problems appearing e.g. in biology or chemistry the measurement of some variables of the problem are difficult or impossible. Therefore a problem of estimation of the states of a dynamical object on the base of only a few available measurements arises. There are numerous techniques for state estimation developed for specific objectives and/or type of information available.

In this presentation the focus is on a set-based estimation of the states of a dynamical system required for construction of optimal guaranteeing feedbacks. In particular, we aim at the construction of polyhedral approximations of sets of all states consistent with the obtained measurements. A problem of constructing estimates, associated with these approximations, is called an optimal observation problem. This presentation presents numerical methods for solving optimal observation problems for nonlinear dynamical systems. To tackle the nonlinearities two problems are studied: an optimal observation problem for a piecewise linear dynamical system (a piecewise linear approximation of the nonlinear problem) and a quasilinear optimal observation problem (local approximations of nonlinearities). For the piecewise linear observation problem the solution is built on the base of two procedures: linearization of the problem along a feasible trajectory and solution of the linearized problem; and correction of the obtained solution by choice of the optimal times of transition between the domains of linearity. For the quasilinear optimal observation problem an asymptotic method of constructing a suboptimal solution on the base of the optimal solution of a corresponding linear problem is proposed. The asymptotic technique combined with the method for solving piecewise linear problems is the base for a numerical procedure for constructing the state estimates of a general nonlinear system in real-time.

Structured doubling algorithms for Hermitian solutions of algebraic Riccati equations. **Tsung-Min Hwang** (National Taiwan Normal University), Wen-Wei Lin (National Tsing Hua University, Taiwan) IC/CT87/062

In this talk, we propose structured doubling algorithms for the computation of weak Hermitian solutions of continuous/discrete-time algebraic Riccati equations. Under the assumptions that partial multiplicities of purely imaginary and unimodular eigenvalues (if any) of the associated Hamiltonian and symplectic pencil, respectively, are all even, we prove that the developed structured doubling algorithms converge to the desired Hermitian solutions globally and linearly. Numerical experiments show that structured doubling algorithms perform efficiently and reliably.

Optimizing system performance in the event of feedback failure. **Debraj Chakraborty** (University of Florida, USA), Jacob Hammer (University of Florida, USA) IC/CT4764/062

Feedback is often used to overcome the adverse effects of perturbations and uncertainties on the performance of engineering systems. However, failures of the feedback channel cannot be completely avoided. The present talk addresses the questions of how and for how long can desirable performance of a perturbed system be maintained after a failure of the feedback channel. In mathematical terms, these questions translate into an optimal control problem which can be formulated as follows.

Let Σ_ϵ be a system that is subject to a perturbation ϵ in its parameters. The exact value of the perturbation ϵ is not known; it is only known that ϵ is bounded by a given constant δ. Now, let $u(t)$ be an input function of Σ, and let $\Sigma_\epsilon u$ be the response of the perturbed system to the signal $u(t)$. The nominal system is Σ_0, and the nominal response to the signal $u(t)$ is $\Sigma_0 u$. Therefore, the deviation in the response caused by the perturbation is $\|\Sigma_\epsilon u - \Sigma_0 u\|$. To reduce the perturbation, add a "correction signal" $v(t)$ to the input signal, so that the perturbed response becomes $\Sigma_\epsilon(u+v)$. Then, the new deviation between the perturbed and nominal cases becomes $\|\Sigma_\epsilon(u+v) - \Sigma_0 u\|$. The correction signal $v(t)$ must be independent of the perturbation value ϵ, as the latter is not known.

Let M be the maximal deviation allowed for the response, and let t_f be the time for which $\|\Sigma_\epsilon(u+v) - \Sigma_0 u\| \le M$. Then, the objective is to find a correction signal $v(t)$ that maximizes t_f, given only that the perturbation ϵ is bounded by δ. The talk presents Euler-Lagrange type first-order conditions for calculating the optimal correction signal $v(t)$. It is shown that, under rather broad conditions, the optimal correction signal $v(t)$ is either a bang-bang signal or can be arbitrarily closely approximated by a bang-bang signal.

An optimal control approach to nonrigid image registration. **Georg Stadler** (University of Texas at Austin, USA), Omar Ghattas (University of Texas at Austin, USA) IC/CT4584/061

Non-rigid image registration can be described briefly as follows: given so-called template and patient images, one wishes to find a reasonable transformation that makes the transformed template as similar as possible to the patient image. Image registration problems are particularly prevalent in medical image processing applications, for example registration of preoperative and intraoperative image-guided surgical plans, finding anatomical aberrations among populations of patients, tracking tumor morphology over time, and cardiac motion analysis. The problem of finding a reasonable transformation is ill-posed and is usually treated by appropriate regularization. While elastic strain energy regularization is often used, we reformulate the registration problem as an optimal control problem. This allows the choice of a regularizer that acts mainly in directions tangential to interfaces within the image. Since these directions lie in the kernel of the Hessian, the minimizer (i.e., the registered image) becomes (almost) independent of the regularization weight parameter. To solve the resulting constrained optimization problems numerically, we apply an inexact Gauss–Newton method. A multilevel approach is used to speed up the iteration and to avoid local minima. The proposed methods are numerically compared with elastic registration. We also discuss the regularity of the transformation between template and patient image, since this is of importance in most applications.

IC/CTS4672/06: NLP algorithms.

Organiser: Nataša Krejić (University of Novi Sad, Yugoslavia)

Linear semi-definite programs with log*-determinant terms.* **Mituhiro Fukuda** (Tokyo Institute of Technology, Japan) IC/CT4370/063

The new version of SDPA permits one to solve linear semidefinite programs with log determinant terms with different nonnegative weights. Such features are already included in SDPT3 and partially in MAXDET. Examples of such problems arise in robust optimization, statistics, quantum information theory, etc. Numerical experiments on test problems will be presented to test its robustness and efficiency in order to attend the demand of further applications.

Convex separable minimization with box constraints. **Stefan Stefanov** (Neofit Rilski South-Western University, Bulgaria) IC/CT379/063

Consider minimization problems with a convex separable objective function subject to a convex separable inequality constraint of the form " $\le$ " / linear equality constraint / linear inequality constraint of the form " $\ge$ ", and bounds on the variables (box constraints). Denote these three problems by $(C^{\le})$, $(C^{=})$, and $(C^{\ge})$, respectively. Problems of the considered form arise, for example, in allocation of resources, in inventory control, in scheduling theory, in facility location, in the theory of search, in implementation of projection-type methods when the feasible regions are the same as the feasible regions of the considered problems, etc. For each of problems $(C^{\le})$ and $(C^{=})$, a necessary and sufficient condition is proved for a feasible solution to be an optimal solution to the respective problem, and a sufficient condition is proved for a feasible solution to problem $(C^{\ge})$ to be an optimal solution to this problem. Algorithms of polynomial complexity for solving the three problems are proposed and convergence of these algorithms is proved. Some particular problems of the forms $(C^{\le})$, $(C^{=})$, and $(C^{\ge})$ as well as computational results are presented.

Newton and Halley are one step apart: a review of computational issues for cubically-convergent methods. **Trond Steihaug** (University of Bergen, Norway), Geir Gundersen (Universitetet i Bergen, Norway) IC/CT2219/063

In this talk we discuss the relationship betweeen Halley's and Newton's methods for unconstrained optimization. Halley's method actually is a class of methods all parameterized with a real parameter α. For unconstrained optimization, Halley's method uses second (the Hessian matrix) and third derivative (called the tensor). When the problem is large the second derivative will be sparse. We introduce the concept of *induced sparsity structure of the tensor*, induced by the structure of the Hessian matrix. We show how to utilize this structure to increase the efficiency. We compare the number of arithmetic operations of Halley's and Newton's method and illustrate the effect of utilizing the sparsity. We also give some numerical results of Halley's method.

Gutiérrez and Hernandez defined a class of methods defined by

$$x_{k+1} = x_k - \{I + \tfrac{1}{2}L(x_k)[I - \alpha L(x_k)]^{-1}\}(F'(x_k))^{-1}F(x_k), \quad k \ge 0,$$

where $L(x) = (F'(x))^{-1}F''(x)(F'(x))^{-1}F(x)$, for solving the nonlinear system of equations $F(x) = 0$.

An equivalent formulation is

$$\begin{aligned} F'(x_k)s_k^{(1)} &= -F(x_k), \\ (F'(x_k) + \alpha F''(x_k)s_k^{(1)})s_k^{(2)} &= -\tfrac{1}{2}F''(x_k)s_k^{(1)}s_k^{(1)}, \\ x_{k+1} &= x_k + s_k^{(1)} + s_k^{(2)}, \end{aligned}$$

which, for $\alpha = 1$, W. Werner observed is two steps of Newton's method applied to the second-order Taylor approximation $T(s) = 0$:

$$F(x+s) \approx T(s) \equiv F(x) + F'(x)s + \tfrac{1}{2}F''(x)ss.$$

Quasi-Newton methods with line search for stochastic optimization. **Nataša Krejić** (University of Novi Sad, Yugoslavia), Zorana Lužanin (University of Novi Sad, Yugoslavia) IC/CT824/063

We introduce a modification of quasi-Newton methods with line search used in deterministic unconstrained optimization problem to the stochastic unconstrained optimization problem. The basic idea is to use the modifications of quasi-Newton equation and line search algorithms. Practical implementation guidance and a nontrivial numerical experiments are presented.

Newton-like method for non-smooth functions with stochastic approximation. **Sanja Rapajić** (University of Novi Sad, Montenegro and Serbia) IC/CT823/064

Various methods for solving nondifferentiable problems have been developed in recent years. Most of them are based on generalized derivatives or smooth approximation of the original function. Applications of stochastic approximation algorithms to nonsmooth functions is one way to overcome difficulties arising from nonsmoothness. A Newton-like method with stochastic approximation, which is a generalization of some method for smooth functions, is proposed.

On the secant method under generalized Lipschitz conditions for the divided difference operator. **Stepan Shakhno** (Lviv National University, Ukraine) IC/CT606/015

In work[1] for investigation of Newton's method for solving nonlinear equations generalized Lipschitz conditions for the derivative operator are suggested. There instead of constant L is used some positive integrable function.

In this work we introduce for the first time the generalized Lipschitz conditions for the divided difference operator. A positive integrable function, partial case of which is a usual Lipschitz constant, is suggested. Under the given conditions the convergence of the Secant method for the solving of operator equations in Banach spaces is investigated and the uniqueness ball for the solution is obtained. As the partial case the known results for Lipschitz constants are received. The proposed approach can be applied to the investigating of iterative difference methods of higher orders of convergence[2].

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IC/CTS4663/06: Optimal design.

Organiser: Fernand Pelletier (Université de Savoie, France)
Co-organiser: Wolfgang Achtziger (Universität Dortmund, Germany)

An SQP multigrid solver for finite-deformation contact problems. **Oliver Sander** (Freie Universität Berlin, Germany) IC/CT1649/063

We present a new algorithm for simulating mechanical contact between two elastic bodies undergoing large deformations. The two bodies are modelled by some hyperelastic material law, and the contact conditions are discretized using a dual mortar basis. The resulting constraint nonconvex optimization problem is solved with an SQP trust-region solver using a maximum-norm trust-region. Each inner iteration is a possibly nonconvex quadratic program on a convex set bounded by half spaces. Using a suitable basis transformation of the finite element space, this set can be written as a tensor product. That way, the inner problem can be solved with a monotone multigrid method. The resulting algorithm converges globally to a first-order stationary point. Numerical experiments show multigrid complexity of the inner solver even for non-trivial examples in three space dimensions.

On multigrid optimization for dense estimation of contrast invariant optical flow. **El Mostafa Kalmoun** (Université Cadi Ayyad, Morocco) IC/CT1019/063

We consider the computation of dense optical flow between two images under possible brightness variation. The problem is formulated as a minimization of an energy functional which consists of two weighted terms. The data term is based on a geometrical approach that is invariant to contrast changes. And the regularization term involves total variation norm which preserves motion discontinuities. For fast numerical solution, we develop and compare two approaches of using multigrid in this optimization framework. The first scheme, called TN/MG incorporates a linear multigrid solver in the inner loop of the truncated newton (TN) method to get a direction of descent. The second, called MG/TN, apply directly a multigrid strategy in the outer TN loop, while a preconditioned conjugate gradient is used for the inner loop.

This Work was done in collaboration with V. Caselles and L. Garrido

Optimal trajectories which are tangent to an affine distribution. **Fernand Pelletier** (Université de Savoie, France), Mihai-Emilian Popescu (ISMMA-Bucharest, Romania) IC/CT1572/063

In this work we study the trajectories which are tangent to an affine sub-bundle in the tangent bundle of a manifold and which minimize the *total energy*. We give some characterizations of such *regular* trajectories in terms of control theory and geometrical theory. We also build some sufficient conditions of existence for such curves. These data are also elaborate on details in the context of nilpotent Lie groups. Finally, these results are applied to a problem of elastic rod's deformations.

Global optimization of truss topology with discrete bar areas. **Wolfgang Achtziger** (Universität Dortmund, Germany), Mathias Stolpe (Danmarks Tekniske Universitet, Denmark) IC/CT1904/063

The talk considers the classical problem of finding a truss design with minimal compliance subject to a given external force and a volume bound. The design variables describe the cross-sectional areas of the bars. While this problem is well-studied for continuous bar areas, we treat here the case of discrete areas. This problem is of major practical relevance if the truss must be built from pre-produced bars with given areas. As a special case, we consider the design problem for a single bar are;, i.e., a 0/1-problem.

In contrast to heuristic methods considered in other approaches, we present an algorithmic framework for the calculation of a global optimizer of the underlying large-scaled mixed integer design problem. This framework is given by a convergent branch-and-bound algorithm which is based on solving a sequence of nonconvex continuous relaxations. The main issue of the of the approach lies in the fact that the relaxed nonlinear optimization problem can be formulated as a quadratic program (QP). Here the paper generalizes and extends theory from the literature. Although the Hessian of this QP is indefinite, it is possible to circumvent non-convexity and to calculate global optimizers. Moreover, the QPs to be treated in the branch-and-bound search tree differ from each other just in the objective function. Together with a special purpose heuristic which quickly finds good feasible discrete solutions, this makes the resulting branch-and-bound method very efficient. The talk closes with several large-scale numerical examples. To the knowledge of the authors, these examples are the largest discrete topology design problems solved by means of Global Optimization.

Zero-level pricing, universal property, and CARA utility functions. **Sy-Ming Guu** (Yuan Ze University, Taiwan) IC/CT4241/063

Zero-level pricing method has been proposed to provide price information when the no-arbitrage pricing method yields a wide price interval in an incomplete market. Zero-level price usually depends on the utility function and investor's initial wealth. Luerberger showed that if investor's utility function is quadratic, then the zero-level price is universal, namely, independent of his/her initial wealth and parameters of the quadratic utility function. In this talk, we show that CRRA utility function has the universal property as well.

Interior-point methods applied to the AC active-reactive optimal power-flow problem using cartesian coordinates. **Roy Wilhelm Probst** (Universidade Estadual de Campinas, Brazil), Aurelio Oliveira (Universidade Estadual de Campinas, Brazil), Secundino Soares (Universidade Estadual de Campinas, Brazil), Adriano Thomaz (Universidade Estadual de Campinas, Brazil) IC/CT2488/063

The primal dual interior point methods are developed to the AC active and reactive optimal power flow problem. The representation of the tensions through cartesian coordinates is adopted, once the Hessian is constant and the Taylor expansion is accurate for the second order term. The advantage of working with polar coordinates, that easily model the tension magnitudes, lose importance due to the efficient treatment of inequalities proportionated by the interior point methods. Before the application of the method, the number of variables of the problem is reduced through the elimination of free dual variables. This elimination does not modify the sparse pattern of the problem. The linear system obtained can be further reduced to the dimension of twice the number of buses also with minor changes in the sparse structure of the matrices involved. Moreover, the final matrix is symmetric in structure. This feature can be exploited reducing the computational effort per iteration. Computational experiments for IEEE systems problems are presented for several starting point strategies showing the advantages of the proposed approach.

IC/CTS4666/06: Discrete optimization.

Organiser: Chuangyin Dang (City University of Hong Kong)

Lessons of distribution processes: what have we learned?. **Nijole Simeliene** (Forschungsverein Litauen, Lithuania) IC/CT579/006

Changes in social and political values have altered the economic and financial environment in which many consumers operate. The management and control of their exposure to the various types of risk have become essential to managing the financial soudness and viability. The traditional profit functions of managing corporate cash positions have become more complex. Many of investment policy developments have emerged over recent years to meet the critical needs for more sophisticated and flexible tools of asset and liability management. This study provides an optimization of distribution processes. We investigate variuos commodity bundles or currency to be distributed among the consumers. Modelling of distribution processes yields to some statements concerning profit functions. Choosing the class of functions, satisfying all reasonable looking conditions has been analyzed.

Determining the optimal production policy for the system with imperfect production . **Chuang-Chun Chiou** (Da Yeh University, Taiwan) IC/CT962/066

This paper presents an extended economic production quantity (EPQ) model with imperfect production, quality scan, rework, and backlog. In this model, a random defective rate is considered, and the production followed by a quality scanning process produces defective items. The scanning process distinguishes the repairable and scrap portion from the defective. Then, the rework starts when scanning process ends. We assume that not all of the repairable items can be reworked to meet the specified quality standard. Some defective items can be restored as normal items, other results in scrap due to repair failure, and the others can be repaired as quality in-between. In the proposed model, the relevant costs consist of the costs for defective reworking, holding, scanning, and disposing the scrap. The optimal operating policy that minimizes the total relevant cost per unit time for the proposed model under the effect of imperfect quality is derived where shortages are allowed and backlogged.

Mathematical programming in decentralized (or hierarchical) decision systems. **Semu Mitiku Kassa** (University of Addis Ababa, Ethiopia) IC/CT514/066

In business and many other practical activities decision making has changed over the last decades. From a single person (the Boss!) and a single criterion (e.g. Profit), decision environments have developed increasingly to become multi-person and multi-criteria and even multi-level (or hierarchical) situations. In organization with hierarchical (or decentralized) decision systems, the sequential and preemptive nature of the decision process makes the problem of selecting an optimum strategy and action very different from the usual operations research methods. Therefore, a multilevel programming approach is considered in modelling such problems.

A multilevel programming problem partitions control of the

decision variables among several decision makers, each acting in a sequence to maximize his/her own objective function. The general framework of the multilevel mathematical programming methods will be discussed in brief detail. Especially the solution method for three-level linear programming problem and its difficulties will be presented.

An arbitrary starting simplicial algorithm for computing an integer point of a class of polytopes. **Chuangyin Dang** (City University of Hong Kong) IC/CT4284/066

An arbitrary starting simplicial algorithm is developed for computing an integer point in a polytope given by $P = \{x \mid Ax \leq b\}$ satisfying that each row of A has at most one positive entry. The algorithm is derived from an introduction of an integer labeling rule and an application of a triangulation of the space and consists of two phases, one of which forms a variable dimension algorithm and the other a full-dimensional pivoting procedure. Starting from an arbitrary integer point in the space, the algorithm leaves the point along one of $n+1$ rays, interchanges from one phase to the other if necessary, and follows a finite simplicial path that either leads to an integer point in the polytope or proves no such point exists. Numerical results show that the algorithm is efficient.

A hybrid model for unique shortest-path routing. **Changyong Zhang** (University of Southern California, USA) IC/CT877/066

Shortest path routing protocols are the most commonly used IP routing protocols. Due to the complexity of the constraints involved, the unique shortest path routing problem has not been explicitly formulated. Existing methods solve the problem heuristically and result in local optima in general. In this talk, two complete and explicit formulations with polynomial number of constraints are first developed, with the aim of finding a global optimal solution to the MIP problem on average data instances arising from real-world application. The two formulations are mathematically equivalent. Based on the investigation of the constraint structures of the formulations, a decomposition algorithm is proposed to solve the problem. The tradeoff is further studied between the efficiency to solve the maser problem at each iteration and the convergence rate of the proposed algorithm. The problem is thereby formulated as a hybrid model by combining the advantages of both the original two models.

Globalising the pattern-search method. **Montaz Ali** (University of the Witwatersrand, South Africa) IC/CT4436/067

The Pattern Search is a direct search based local optimization method. In this research the author proposed a global optimization algorithm that combines the salient features of Pattern Search, Simulated Annealing and Multilevel Single Linkage in a single framework. Results are presented which show that the new algorithm is very efficient and robust.

06: Optimization, Posters

IC/PP1948/006: **Inverse heat-transfer problems with differential objective function.**

Presenter: Andrzej Wawrzynek (Silesian University of Technology, Gliwice„ Poland)

To search a solution of inverse heat transfer problems an objective function is usually used. The function is a sum of squares of differences between two temperatures: the temperature, which is measured in some given measuring points and the calculated one. The matter of modifications of this objective function consists in introducing of weighting coefficients for measuring points or using some additional information results from physical analysis of the investigated problem. In this paper a new approach is presented: from N measuring points we choose one point (basic measuring point). Two sets of temperature differences are created: the first one consists of differences between two temperatures - in the given and basic points; the second set is a set of the same differences of temperature but the calculated ones. Design parameters (DP) are found from the condition of existence of objective function extreme. The objective function (OF) consists of squares of differences of adequate - measured and calculated - differences from the two described sets. A new OF is called Differential Objective Function (DOF) to distinguish from the classical OF. For transient problems, in all time steps the basic temperatures are different; so the DOF could not be created by a simple change of variables. There were investigated several series of inverse hest transfer problems with simulated measures with infrared camera to compare the both objective functions. It was assumed that laboratory specimen was a cylinder of concrete. The transient problems described by 4 parameters were solved. Several kinds of measuring errors were taken into consideration. In some cases of the errors solutions with the DOFun are exact and simultaneously the OF generates solutions with large errors. Generally, the DOF for transient heat transfer problems leads to better solutions then the classical DO. For all analysed problems the sensitivity coefficient method was applied to find the minimum value of the OF.

IC/PP4715/010: **Avoiding a random barrier as long as possible.**

Presenter: Mario Lefebvre (École Polytechnique de Montréal, Canada)

Let $x(t)$ be a one-dimensional diffusion process. Suppose that $x(t)$ evolves between a reflecting boundary at $-D$, and an absorbing boundary at $+D$. We want to maximize the time spent by the controlled process in the interval $[-D, D)$, where D is a random variable, while taking the quadratic control costs into account. The optimal control is found by considering the uncontrolled process that corresponds to $x(t)$. This problem is an extension of what is known as LQG homing.

IC/PP638/010: **Control suboptimal linear systems with delay and application in halieutics.**

Presenter: Baghdadli_Dib Nabahats Adiba (University of Tlemcen Algeria)

In this paper, we present a method under optimal for the determination of optimal control of the linear systems at delay, then applied we it to halieutics, by considering a total model that the specialists generally use it in this field, then we sought to control fishing, so as to reduce the fluctuations of the capture and the effort of fishing what brings back to us to a problem of optimal control of a system to delay with a quadratic criterion, then by using the method under optimal we could solve this problem numerically.

IC/PP1406/010: A note about self-dual k-out-of-n systems.

Presenter: Maria Albina Puente (Universitat Politècnica de Catalunya, Spain)
Co-author: Francesc Carreras (Universitat Politècnica de Catalunya, Spain)
Co-author: Josep Freixas (Universitat Politècnica de Catalunya, Spain)

We consider here a class of k-out-of-n systems and study the variation of their reliability under different assumptions. It shown that a way to achieve highly reliable self-dual k-out-of-n systems consists in maintaining the reliability of the components at a level of performance above ¡.

The k-out-of-n systems consist of n components of the same kind. The system works if at least any k of its n components are operating. Particular cases of these systems are parallel and series systems, corresponding to k=1 and k=n, respectively. Applications of k-out-of-n systems can be found in the areas of target detection, communication, safety monitoring systems and, particularly, in the area of voting systems.

In this work we study the reliability of the self-dual k-out-of-n systems, when it is assumed that all components have the reliability, p. We especially focus on the variation of the system reliability under two assumptions: (i) if we slightly increase the component reliability p and (ii) if we increase the number of components of the system. We also compare the system reliability with the components reliability.

In practice, design problems can vary appreciably if we add restrictions and the design process may consider more complex system configurations. We study the case with multiple self-dual k-out-of-n systems.

IC/PP4886/061: Optimal design and optimal damping set to a hyperbolic problem.

Presenter: Faustino Maestre (Universidad de Castilla-La Mancha, Spain)

In this work we analyze a 2D optimal design problem governed by a linear damped 1D wave equation. In this problem we would like to find simultaneously the best time-dependent optimal layout of two isotropic materials and the static position of the damping set in order to minimize certain non-linear cost depending on the gradient of the state. By means of the gradient Young measures, we compute a full relaxation of the original optimal design problem (since the lack of classical solution of these non-linear optimization problems is typical). This relaxation is justified by the presence of optimal microstrutures, first-order laminates associated to the material design and the damping set. All these analytical computations are contrasted with numerical experiments.

IC/PP718/062: Guaranteed optimization of uncertain systems with application for energy security assessment.

Presenter: Natalia Balashevich (National Academy of Sciences, Belarus)
Co-author: Faina Kirillova (National Academy of Sciences, Belarus)

A control system affected by unknown but bounded disturbances is considered. The aim is to construct a feedback such that a closed system reaches a convex endpoint set in a fixed time and to provide a maximal guaranteed value of an endpoint performance index. To account available information on disturbances, the concept of closable feedback is introduced [1]. This type of feedback is defined on the base of the assumption that the system's states will be known at some future instants. The more such closure instants are used, the better guaranteed value of the objective function could be achieved. However the increase of the number of closure instants causes enormous computational efforts. So the problem is to choose the optimal positions of a fixed number of closure instants.

Before the beginning of control process optimal positions of closure instants for given bounds of disturbance are identified and optimal open-loop control is constructed. Then, in the course of control process these positions are corrected in accordance with realized system's states, values of feedback are computed and fed to the system's input. Algorithms of solving auxiliary problems and implementing a closable feedback are elaborated.

The suggested scheme is used for optimization of economic growth model subject to constraints characterizing the desired level of energy security indicators [2]. The goal is to provide sustainable development of economic system in the face of uncertainty in energy supplies and prices.

[1] Gabasov R., Kirillova F., Balashevich N. Guaranteed on-line control for linear systems under disturbances // Func. Diff. Equ., 2004, 341-361.

[2] Mikhalevich A.A. State and directions of strengthening energy security of the Republic of Belarus // Proc. Int. Conf. "Energy of Moldova 2005", Chisinau, 2005, 54-59.

IC/PP3655/062: Optimal-control problem of some hemi-variational inclusion: convergence of Galerkin approximation.

Presenter: Andrzej Just (Technical University of Lodz, Poland)

In this paper we study the optimal control problem described by a hemivariational parabolic inclusion. We derive the existence of optimal solutions. Then we prove the convergence of optimal values for approximated control problems to the one for the original problem. Finally, we give a simple example.

IC/PP3407/063: Application of non-local optimization approaches for synthesis of multilayer optical systems.

Presenter: Svetlana Sharapova (Moscow State University, Russian Federation)

The dependence of the spectral coefficients of layered medium on its parameters (thickness and refractive index of each layer) allows one to pose the inverse problem of searching the parameters of the medium with the desired spectral characteristics, called also the problem of synthesis of optical coatings. The characteristic feature of inverse synthesis problems is that the uniqueness of the solution is not essential. Modern approaches for the design of multilayer systems generally allow sufficiently good solution to be obtained. Therefore the question becomes of constructing not just one, but a set of essentially different designs with approximately identical spectral characteristics. With this goal, two new approaches are proposed, both based on the numerical methods of non-local optimization.

The first approach is based on the random choice of an initial approximation and the consequent application of optimization methods for the searching the local extremum of the problem. The best extremum, in the sense of the criterion func-

tion, is chosen as a solution. Different local zero- and first-order optimization methods are applied and compared in effectiveness. The results showed that the zero-order methods do not provide satisfactory effectiveness, whereas first-order methods could be used to solve different problems.

In the second approach, genetic algorithms were used for the optimization of the problem. Genetic algorithms perform a class of global search methods which are patterned on the theory of evolution. They are stochastic algorithms, which search the solution space by operating not on a single solution, but on a population of candidate solutions. This approach also shows to be very effective, and some model problems arising in the synthesis of multilayer optical systems (antireflection coating and beam splitter syntheses) have been solved by means of the proposed method.

IC/PP1265/063: Distance evaluation between quadric surfaces in $\mathbb{R}^n$.

Presenter: Marina Yashina (Saint Petersburg State University, Russian Federation)
Co-author: Alexei Uteshev (Saint Petersburg State University, Russian Federation)

Given the equations of the quadrics in $\mathbb{R}^n$, namely $X^T\mathbf{A}_1X + 2B_1^TX - 1 = 0$ and $X^T\mathbf{A}_2X + 2B_2^TX - 1 = 0$, we solve the distance evaluation problem via reducing it to that of evaluation of the minimal positive root of a univariate algebraic equation. This is performed via application of the Elimination theory algorithms. For instance, for the centered surfaces one has:

Theorem. The distance between ellipsoids $X^T\mathbf{A}_1X = 1$ and $X^T\mathbf{A}_2X = 1$ equals zero iff the matrix $\mathbf{A}_1 - \mathbf{A}_2$ is not sign-definite. Otherwise, the square of the distance coincides with (in the general case minimal) positive zero of the polynomial

$$\mathcal{F}(z) = \mathcal{D}_\mu(\det(\mu\mathbf{A}_1 + (z-\mu)\mathbf{A}_2 - \mu(z-\mu)\mathbf{A}_1\mathbf{A}_2)).$$

Here $\mathcal{D}$ stands for the discriminant of the polynomial treated w.r.t. the indicated variable.

In the frame of this approach, the corresponding nearest points on the considered surfaces can be determined as well.

IC/PP553/064: A kernel function based interior-point methods to solve $P_*(k)$-linear complementary problem.

Presenter: Mohammad Reza Peyghami (K.N. Toosi University of Technology, Iran)

Kernel functions play a special role among interior-point algorithms for linear complementary problems to define a new search direction. In this paper, an interior point algorithm based on a new class of kernel functions is proposed to solve the $P_*(k)$-linear complementary problem, $k \geq 0$. Using some appealing properties of new kernel functions, we prove that the new kernel function based large-update primal-dual interior point methods for solving $P_*(k)$-linear complementary problem enjoy an $O\left(\frac{1}{q\sqrt{p}}qk\sqrt{n}\,(\log n)^{1+\frac{1}{q}}\log\frac{n}{\varepsilon}\right)$ iteration bound, where $p, q \geq 1$ are the parameters of the new class of kernel functions. In special case, for fixed $q \geq 1$ and $p = O(\log n)$, we obtain the so far best worst case theoretical complexity, namely $O\left(k\sqrt{n}\log n\log\frac{n}{\varepsilon}\right)$, for large-update primal-dual interior point methods to solve $P_*(k)$-linear complementary problem.

IC/PP1978/065: LSTRS: Matlab software for large-scale trust-region subproblems and regularization.

Presenter: Marielba Rojas (Danmarks Tekniske Universitet, Denmark)
Co-author: Sandra Santos (Universidade Estadual de Campinas, Brazil)
Co-author: Danny Sorensen (Rice University, USA)

We describe a Matlab implementation of the method LSTRS for the large-scale trust-region subproblem:

$$\min \tfrac{1}{2}x^THx + g^Tx \quad \text{subject to } \|x\|_2 \leq \Delta,$$

where H is an $n \times n$, real, large, symmetric matrix, g is an n-dimensional real vector, and Δ is a positive scalar. This problem arises in connection with the trust-region globalization strategy in optimization. A special case, namely, a least-squares problem with a norm constraint, is equivalent to Tikhonov regularization for discrete forms of ill-posed problems.

LSTRS is based on a reformulation of the trust-region subproblem as a parameterized eigenvalue problem, and consists of an iterative procedure that finds the optimal value for the parameter. The adjustment of the parameter requires the solution of a large-scale eigenvalue problem at each step. The method relies on matrix-vector products only and has low and fixed storage requirements, features that make it suitable for large-scale computations. In the Matlab implementation, the Hessian matrix of the quadratic objective function can be specified either explicitly, or in the form of a matrix-vector multiplication routine. Therefore, the implementation preserves the matrix-free nature of the method. The Matlab implementation offers several choices for the eigenvalue calculation and it also allows the users to specify their own eigensolver routine.

We present a brief description of the LSTRS method and describe the main components and features of the Matlab software. We include comparisons with state-of-the-art, large-scale techniques for the problem. We present examples of use of the software as well as results from the regularization of large-scale discrete forms of ill-posed problems.

IC/PP4872/066: Determination of shortest paths in fuzzy weighted networks.

Presenter: Pijus Kanti De (Banasthali Vidyapith, India)

Computation of shortest path play an important role in all transportation problems and also it is an archetypical problems encountered in the domain of combinatorial optimization. Shortest path problem is the most common problem among all types of optimum path problems. Fuzziness in a network can be introduced in many different ways e.g. through edge weights, edge capacities, vertex restrictions, or arc lengths etc. In this problem author has tried to review and formalize the recently developed fuzzy shortest path problems. In the present problem attempt has been made to study the shortest path in a network in which edge weights have been considered as uncertain-that means either imprecise or unknown. Triangular fuzzy numbers have been used to represents these uncertain edge weights and then defuzzification has been done by applying signed distance ranking method to calculate fuzzy shortest path. A dynamic programming recursion formula and a tabular calculation method have been used to solve this problem.

IC/PP4060/066: Quasi-independence space and greedy spaces.

Presenter: Anil Pedgaonkar (Sydenham College, Mumbai, India)

We introduce the notion of a quasiindependence space. This is a unification of the concept of matroid and polymatroid (Introduced by Jack Edmonds). The concept serves to illustrate that viewed in this angle polymatroid is the complete continuous analogue of the notion of matroid. We claim that we distinguish between two rank functions, namely set rank function (defined for ground set and it's subsets) and vector rank function. We have also introduced two definitions of quasiindependence space using independent vectors and proved equivalence of all definitions. We have used a tool called a set W which is defined by putting some conditions on W. We are able to give a unified treatment for both discrete and continuous notions. The notion clarifies many aspects of greedy algorithms in a matroid setting and also allows us to study integer polymatroids. Moreover we are soon led to the notion of greedy space or semigreedy space a continuous analogue of the notion of greedoid introduced by Lovasz. This notion is defined and some optimization results are obtained. For Matroid theory we refer to the text of D.J. Welsh, (Matroid theory) listed in the references.

We have rephrased and proved the necessary and sufficient condition for greedy algorithm in the context of quasiindependence spaces.

IC/PP4696/066: Adding an edge between two levels to a complete K-ary tree minimizing total path length.

Presenter: Kiyoshi Sawada (University of Marketing and Distribution Sciences, Japan)

This study considers addition of relation to a pyramid organization structure such that the communication of information between every member in the organization becomes the most efficient. The pyramid organization structure can be expressed as a rooted tree, if we let nodes and edges in the rooted tree correspond to members and relations between members in the organization respectively. This presentation proposes a model of adding an edge between two nodes with different depths to a complete K-ary tree $(K = 2, 3, \cdots)$ of height H $(H = 2, 3, \cdots)$. When a new edge between a node with a depth M and its descendant with a depth N is added, an optimal pair of depth $(M, N)^*$ is obtained by maximizing the total shortening path length which is the sum of shortening lengths of shortest paths between every pair of all nodes. The optimal pair of depth $(M, N)^*$ is given as follows. When $K = 2$, then $(M, N)^* = (0, 2)$ for $H = 2, 3, 4, 5$ and $(M, N)^* = (0, 4)$ for $H = 6, 7, \cdots$. When $K = 3, 4, \cdots$, then $(M, N)^* = (0, 2)$, irrespective of H.

IC/PP3403/066: Integer optimization in WDM-filter synthesis problems.

Presenter: Dmitry Sharapov (Moscow State University, Russian Federation)

From a physical point of view, any wavelength-division multiplexing (WDM) filter is a resonance structure formed by multilayer mirrors and cavities connected with spacer layers. The total number of WDM filter layers may exceed 100, but the number of design parameters is much smaller. The spectral transmittance of a WDM filter depends on the number of filter cavities, the reflectance of filter mirrors and the phase properties of filter cavities. Successful manufacturing of WDM filters is possible due to the thickness errors self compensation provided by turning point optical monitoring. This type of monitoring needs the optical thicknesses of filter layers to be multiples of a quarter-wave at the central wavelength. The reflectance of a quarter-wave mirror depends on the number of mirror layers, and the phase properties of cavities are also defined by an integer parameter. Therefore, all design parameters take only specific integer values. It is possible to design WDM filters by a direct computation of spectral characteristics for different combinations of design parameters. However, the number of possible combinations is actually too large to produce a satisfactory design. In order to obtain a good initial approximation one can use ideas from classical approaches.

The inverse problem of designing multilayer coatings lies in searching the parameter system which satisfies the desired optical specifications. The performance of a WDM filter at any stage of the design is measured by the value of a merit function. Designing WDM filters can be considered as a specific integer optimization problem, where the main design parameters are the numbers of layers of filter mirrors and the orders of spacers. Considered classical design ideas enable the designer to interactively specify a filter prototype that can be then optimized to meet all design requirements. We propose two integer optimization techniques proved to be very efficient for constructing different filter designs.

07: Discrete Mathematics, Minisymposia

IC/MP94/015: Tensegrities.

Organiser: Brigitte Servatius (Worcester Polytechnic Institute, USA)
Co-organiser: Ileana Streinu (Smith College, USA)

Tensegrities, or tensed frameworks, are objects that fit well in the domain of metric geometry and combinatorics. Questions of rigidity and stability were already asked by architectural designers like Fuller and Emmerich and also by the artist Snelson in the 1960s and 1970s. Key results and conjectures of that time are compiled in Branko Grünbaum's *Lectures in lost mathematics*. Recent mathematical progress has paved the way to new applications in the biological sciences as well as in structural engineering. This minisymposium is intended to communicate this progress to researchers in the fields of mathematics, computer science, biology, and mechanical engineering.

Symmetric tensegrities. **Robert Connelly** (Cornell University, USA) IC/MT4495/015

Tensegrities come in all kinds of shapes and forms with all kinds of applications and purposes. Often the calculations to determine their stability can difficult or unwieldy. But if it is symmetric enough, the symmetry can be used to simplify and clarify the situation. Many of the tensegrities constructed by artists are highly symmetric, and it can be shown that they are prestress stable in the sense of structural engineering.

Combinatorial conditions for the rigidity of tensegrity frameworks. **András Recski** (Budapest University of Technology and Economics, Hungary) IC/MT4197/015

A graph is called rigid in the d-dimensional space if the bar-and-joint frameworks corresponding to its generic embeddings in the d-dimensional space are rigid. Rigid graphs are just the connected ones for $d = 1$; they were characterized by Laman and Lovász–Yemini for $d = 2$, their characterization for $d > 2$ is basically open.

One can generalize this decision problem for tensegrity frameworks in two different ways. In the weak version we are given a graph and we have to decide whether there are tensegrity frameworks (with appropriate tripartition of the edge set of the graph for bars, cables and struts) which are rigid in the d-dimensional space. In case of the strong version the input consists of the graph and the tripartition and we have to decide whether there are tensegrity frameworks with this tripartition of the edge set, which are rigid in the d-dimensional space.

We give polynomial algorithms for both the weak and the strong versions for $d = 1$ (joint result with O. Shai) and for the weak version for $d = 2$. In case of $d = 2$ some partial results related to the strong version will also be presented.

Tensegrity and symmetry. **Simon Guest** (University of Cambridge, UK) IC/MT4848/015

This talk will describe the links between group representation theory and tensegrity structures. Tensegrity structures are generally non-generic: commonly they will either have some non-trivial geometric symmetry, or an affine transformation will take them to a symmetric configuration. Group representation theory is commonly used in the applied sciences, and particularly Chemistry, to study symmetric objects: here, I will describe how the ideas developed in Chemistry can be applied to the study of tensegrity structures. In particular, I will describe how the 'form-finding' problem can be simplified by using group representation theory, and will connect these ideas to Bob Connelly's catalogue of symmetric tensegrities.

IC/MP171/015: Mathematics of VLSI design.

Organiser: Jens Vygen (Universität Bonn, Germany)
Co-organiser: Juergen Koehl (International Business Machines (IBM), Germany)

VLSI design is one of the most attractive application areas of discrete mathematics. Key features are the variety of interesting and well-defined optimization problems, constantly new problems due to rapidly progressing technology, huge and exponentially growing instance sizes, and the economic relevance.

In the last decades, more and more techniques from combinatorial optimization have been applied, and challenging problems from industrial practice led to new, and sometimes deep, mathematical theory and new algorithms. Strong relationships between academia and industry enable research focus on the key challenges and enable industry to use new research results directly. Most complex chips cannot be designed anymore without this interplay.

This minisymposium will cover key mathematical achievements in almost all areas of VLSI design, from the architecture of switching networks and logic optimization problems to timing closure, clock design problems, and classical layout, including design-for-manufacturability aspects that become very important for $65\,\mathrm{nm}$ and $45\,\mathrm{nm}$ technologies.

Physical design of digital ASICs: an overview. **Matthias Ringe** (International Business Machines (IBM), Germany) IC/MT3921/015

Physical design is the process of turning a structural description of a design into geometric data that will be used for manufacturing. Compared to processors the physical design of application specific integrated circuits (ASICs) is typically more automated and provides interesting challenges. The first part of the talk will present an overview of the design steps involved including placement, timing optimization, clock tree construction, wiring, and sign-off.

A particularly interesting problem is placement since being an early design step it has high impact on all following steps. The talk will give an introduction to standard cell placement, floorplanning, and legalization.

Integrated-circuit design: mathematical techniques for dealing with variations. **Ulf Schlichtmann** (TU München, Germany) IC/MT3927/015

After decades of relentlessly shrinking the sizes of transistors and wires, today the semiconductor industry can combine billions of transistors on a single integrated circuit (IC). This achievement comes at a cost, however. As the device dimensions have decreased, the ability to accurately control these dimensions during manufacturing has decreased as well. The industry is confronted with increasing variations of parameters such as transistor dimensions, in some cases of more than 25% of their nominal value. To ensure that despite such significant variations, a high percentage of manufactured ICs will fulfill their specifications, mathematical techniques are increasingly used during the development of ICs to analyze the impact of manufacturing variations and to optimize the IC design for robustness against such variations. We will present such techniques and discuss recent research results.

Timing optimization of VLSI designs. **Stephan Held** (Universität Bonn, Germany) IC/MT3461/015

Timing optimization is one of the key problems in VLSI design. Many different methods (i.e., transistor sizing, repeater-tree construction, clock-skew scheduling, logic restructuring) are combined to meet extremely tight timing constraints. A wide spectrum of methods from combinatorial optimization as well as nonlinear programming is applied in these subproblems. Increasing instance sizes made many classical approaches inoperative due to long run-times. We introduce new algorithms for selected sub-problems which helped to reduce run-times from several days to a few hours on largest industrial instances.

Design of robust signal and clock networks. **Philipp Panitz** (Universität Hannover, Germany), Markus Olbrich (Universität Hannover, Germany), Erich Barke (Universität Hannover, Germany) IC/MT3821/015

As technology scales down into the nanometer region new design challenges emerge. Wire delays become the performance bottleneck in VLSI circuits. Copper is introduced as new wiring material because of its low sheet resistivity, hence low signal propagation delay. The main defect mechanism shifts from shorts to opens due to the different manufacturing process for copper wires. Open defects limit the functional yield. The parametric yield decreases because of timing uncertainties emerging from manufacturing variation. Clock skew variation becomes critical because it may shorten the cycle length of the critical path. The result is a logical error. The variation of signal nets has to be accounted for. Worst case considerations lead to overly pessimistic designs. Design techniques which reduce the variation of design parameters avoid over design and increase parametric yield.

Whereas tree topologies have been applied due to their minimal wire length, the application of generic routing graphs provides multiple paths to specific sinks. Multiple paths from the source to the sink of the signal increase the robustness against open defects and smoothes the effect of variation. Yield is considered a new design objective, today. New mathematical methods are applied within global routing to create routing graphs instead of routing trees. As multi-driver nets are created by link insertion into clock nets and new buffering approaches the calculation of signal propagation delays has to be enhanced to handle general networks with multiple inputs. New design techniques and required mathematical methods are the emphasis of this talk.

IC/MP171/015: Mathematics of VLSI design. #2

Organiser: Jens Vygen (Universität Bonn, Germany)
Co-organiser: Juergen Koehl (International Business Machines (IBM), Germany)

(For abstract, see session #1 above.)

Generalizing Dijkstra's algorithm to speed-up VLSI routing. **Sven Peyer** (Universität Bonn, Germany), Dieter Rautenbach (TU Ilmenau, Germany), Jens Vygen (Universität Bonn, Germany) IC/MT3888/015

We generalize Dijkstra"s algorithm to compute shortest paths in huge undirected graphs with non-negative integral edge lengths. The main idea is to cover the vertex set V by l subsets and label these subsets instead of individual vertices. We apply this algorithm to 3-dimensional grid graphs in order to speed up path search in VLSI routing. Two granularities of the sets V_i will be used. In the first application we compute reduced costs for the edges of the routing graph. Here, the subsets V_i are large subgraphs of the given grid graph and we achieve a running time of $O(l \log l)$. Secondly, we apply the algorithm to the detailed path search, where V_i is a set of l intervals covering all vertices. The running time is $O((d+1)l \log l)$, where d is the length of the shortest path w.r.t the reduced costs. This enables us to find millions of exact shortest paths in a graph with billions of vertices in a few hours. Our algorithm is part of BonnRoute, a state-of-the-art routing tool which has been used for almost 20 years to route leading-edge industrial chips.

A speculative transmission scheme for scheduling-latency reduction. **Ilias Iliadis** (IBM Zurich Research Laboratory, Switzerland) IC/MT3536/015

Low latency is a critical requirement in some switching applications, specifically in parallel computer interconnection networks. The minimum latency in switches with centralized scheduling comprises two components, namely, the control-path latency and the data-path latency, which in a practical high-capacity, distributed switch implementation can be far greater than the cell duration. A new speculative transmission scheme is presented to significantly reduce the average control-path latency by allowing cells to proceed without waiting for a grant, under certain conditions. It operates in conjunction with any centralized matching algorithm to achieve a high maximum utilization. An analytical model is presented to investigate the efficiency of the speculative transmission scheme employed in a non-blocking $N \times NR$ input-queued crossbar switch with R receivers per output. Using this model, performance measures such as the mean delay and the rate of successful speculative transmissions are derived. The results demonstrate that the control-path latency can be almost entirely eliminated for loads up to 50%.

Factoring boolean functions and low readability. **Dieter Rautenbach** (TU Ilmenau, Germany) IC/MT3939/015

It is known since a long time that boolean read-once formulas can be characterized using a graph associated to their *sum of products* representation. We discuss, simplify and extend recent related results obtained by Golumbic and Mintz (Factoring logic functions using graph partitioning, ICCAD 1999) and Golumbic, Mintz and Rotics (Factoring and Recognition of Read-Once Functions using Cographs and Normality, DAC 2001).

BonnTools: mathematics for layout and timing closure of complex chips. **Jens Vygen** (Universität Bonn, Germany), Dieter Rautenbach (TU Ilmenau, Germany), Bernhard Korte (Universität Bonn, Germany) IC/MT5018/015

The BonnTools provide innovative solutions for layout and timing closure that are used for many of the most complex integrated circuits. During 20 years of cooperation between the University of Bonn and IBM, new mathematical foundations and algorithms have been developed for the need of new technologies and leading-edge designs.

IC/MP336/072: Complex networks their models and dynamics.

Organiser: Anna Lawniczak (University of Guelph, Canada)

Dynamics of data communication networks, transportation networks, epidemiological, biological, or social networks usually depend on large number of parameters and present a challenging task to study them. Understanding the dependences among parameters and dynamics are important for the prediction purposes, the design of the man-made networks, controls of their dynamics or the controls of the dynamics of naturally occurring networks. Studies of dynamics of complex networks require models development at various levels of networks abstraction, followed by application and/or development of various analytical and statistical methodologies to investigate them. The Minisymposium will review and report on recent progress on mathematical, statistical physics and statistical methodologies to study the dynamics of complex networks of various types. It will report on new results obtained in the investigation of dynamics of complex networks, i.e., synchronization, long range dependence, phase transition. It will explore interdisciplinary cross-fertilization among various application domains.

Automata network models and their applications to study complex dynamics of data-communication networks and spread of epidemics. **Anna Lawniczak** (University of Guelph, Canada) IC/MT3184/0

Dynamics of flow and congestion in data communication networks or of spread of epidemics of infectious diseases in human populations can be complex and often are not well understood. Understanding of these complex dynamics is important for their control, prediction purposes, in data communication networks for their design, or for prevention of spread of epidemics and design of vaccination strategies. In this talk we present microscopic models of automata network types to study these dynamics and we discuss how in both cases the macroscopic dynamics emerge from the microscopic interactions. Using an abstraction of the Network Layer of the ISO OSI (International Standard Organization Open Systems Interconnect) Reference Model, that we developed, we investigate packet traffic dynamics in our data network models of data communication networks of packet switching type. We explore how network connection topology and routing algorithms affect these dynamics, in particular near the phase transition point from free flow to congestion. Also, we present individually based simulation model to study spread of epidemics of SIR (susceptible-infected-removed) type, i.e. influenza epidemics, and present selected simulation results of spatio-temporal dynamics of spread of epidemics for realistic population distribution. Additionally, we explore interdisciplinary cross-fertilization between the two discussed application domains.

Critical phenomena in evolving networks. **Danuta Makowiec** (University of Gdansk, Poland) IC/MT2755/0

The Watts–Strogatz algorithm, which transfers a square lattice to a small-world network, is modified by preferential rewiring. The preference is related to a vertex degree. Evolution of the network is set as two-step: sequential preferential rewiring of edges measured by p and updating the information about the changes made. It appears that the evolving system self-organizes into stationary states. The topological transition in the graph structure is observed with respect to p. Leafy phase: a graph formed by multiple connected vertices (graph skeleton), with plenty of leaves attached to each skeleton vertex, emerges when p is small enough to pretend an asynchronous evolution. Tangling phase: a phase where edges of a graph circulate frequently among low degree vertices, occurs when p is large. Ferromagnetic transition properties will be studied in each of the evolving network's stationary state.

Double-layer dynamics and human migration after catastrophic events. **Monica-Gabriela Cojocaru** (University of Guelph, Canada) IC/MT3713/0

This talk presents a new application of double-layer dynamics theory (DLD) in modelling dynamics of human migration problems reformulated as transportation networks problems. Recent results in DLD allow for generalizing existing migration models by accounting for sudden (discontinuous) changes in migration flows as a consequence of, for example, natural disasters or catastrophic events.

Inferring topological and dynamical properties of immune, genetic and social networks and their relation to technological networks. **Pietro Lio** (University of Cambridge, UK) IC/MT2671/0

In this talk I will show results from the analysis of the dynamical properties of immune system response networks to HIV quasi species infection, risk perception and adaptiveness of social networks in epidemics spreadings and cell-cycle transcriptional networks. Then I will describe how the study of biological networks may inspire current technology in wired and wireless networks.

07: Discrete Mathematics, Contributed Talks

IC/CTS4898/07: **Networks, graphs incl. general.**

Organiser: Radu Serban (Lawrence Livermore National Laboratory, USA)

Macro-additions: a combinatoric algorithm for summations of integers. **Arnaud Lafonte** (Laboratório Nacional de Computação Científica, Brazil) IC/CT4093/010

The purpose of this article is to provide an adequate algorithm for solving the following question: "What is the total sum of all nonnegative integers that can be generated from set of n basic digits of positional number system base λ"? The answer is an algorithm that will enable us to get this sum without having to add the summands in a term-wise mode.

The article begins with the introduction of the concept of *generation-composition* of a set F onto a set G. The result of a generation-composition is a family of sets Q, whose members are strings of $1, 2, \cdots, p$ elements. The elements of set F are p combinatoric-type operators, f_1, f_2, $\cdots$, f_p. The set G is called a *generator set* or *mother-set'*. Its members are n distinct elements: a_1, $a_2, \cdots$, a_n. The elements of resulting sets Q are strings of $j, \cdots, p$ elements each. Based on foundations of set theory, number systems, combinatorics and through a strong algebraic development, the authour obtained the searched algorithm, which was denoted *algorithm of macro-additions*. It provides an easy and fast way to calculate huge sums of integers as are the ones concerning all the integers belonging to the numerical sets that are generated from an *arrangement-type* generation-composition. The algorithm was tested in several numerical examples shown in the

paper; it proved to be an strong time-saving device for those kinds of summaritions.

A theorem on macro-additions is proposed, as well as the concepts of *generator-set* (or *mother-set*), *operator-set* (or *father-set*) and *derived set* (or *son-set*). Suggestions for future search on this matter are also proposed in the paper.

Key-words: discrete mathematics, algorithm, arrangements, combinatorics, generation-composition, sets, strings.

Highly-robust error-correction by convex programming. **Paige Randall** (California Institute of Technology, USA), Emmanuel Candès (California Institute of Technology, USA) IC/CT4261/071

We discuss a stylized communication problem where one wishes to transmit a real-valued signal $x \in \mathbb{R}^n$ (a block of n pieces of information) to a remote receiver. Is it possible to transmit this information reliably when a fraction of the transmitted codeword is corrupted by arbitrary gross errors, and when, in addition, all the entries of the codeword are contaminated by smaller errors (e.g. quantization errors)?

We show that if one encodes the information as Ax where $A \in \mathbb{R}^{m\times n}$ $(m \geq n)$ is a suitable coding matrix, there are two decoding schemes that allow the recovery of the block of n pieces of information x with nearly the same accuracy as if no gross errors occur upon transmission (or equivalently as if one has an oracle supplying perfect information about the sites and amplitudes of the gross errors). Moreover, both decoding strategies are very concrete and only involve solving simple convex optimization programs, either a linear program or a second-order cone program. We complement our study with numerical simulations showing that the encoder/decoder pair performs remarkably well.

A new approach to the 15 puzzle. **Rooholah Majdodin** (Sharif University of Technology, Iran) IC/CT4482/010

In this paper we reexamine the 15 or (n^2-1) puzzle and study its characteristics and solvability by a novel method. Also we introduce an elegant algorithm to solve the puzzle when possible by bringing the tiles to their due squares in any desired order. The defenitions and theorems are as follows:

Definition (2.1) If a sequence of moves is denoted by $\mathbf{S}$, its reverse is denoted by $\mathbf{S}^{-1}$.

Lemma (2.2) If a sequence $\mathbf{S}$ of the special piece moves transforms arrangement $\mathbf{R_1}$ to arrangement $\mathbf{R_2}$, then the reverse of $\mathbf{S}$, denoted by $\mathbf{S}^{-1}$, transforms $\mathbf{R}_2$ to $\mathbf{R}_1$.

Lemma (2.3) Suppose that arrangements $\mathbf{R_1}$ and $\mathbf{R_2}$ are reachable. Then any arrangement $\mathbf{R}_3$ reachable from $\mathbf{R_2}$ is also reachable from. $\mathbf{R_1}$.

Definition (2.4) A simple problem or a simple case is a case that in both of its initial and final arrangements, the special piece is placed in the left lower corner of the checkerboard.

Theorem (2.5) If a simple case has a solution, then the sequence of the special piece moves forms a path consisting of some loops beginning and ending at the left lower corner.

Lemma (2.6) If the path of the special piece forms a loop in the checker bored, it has made an even number of moves.

Definition (2.7) A switch is a change of place of any two pieces located on two specific squares in the checkerboard. An adjacent switch is a switch of two adjacent squares. A piece switch is a change of place of two specific pieces, wherever they are.

Definition (2.8) A tri, is a move in the play ground, consisting of a two succeeding adjacent switches which are perpendicular and share a square. A proper tri is one that does not contain the lower left square of the checker board.

Theorem (2.9) If a simple case is solvable, there is a sequence of tris that transforms the start arrangement to the final arrangement.

Theorem (2.10) If a sequence of piece switches leads to an arrangement that is identical to the initial arrangement, then its length is even.

Theorem (2.11) If in a simple case, the start and final arrangements differ in an odd number of switches (not including the lower left square), it is not solvable.

Theorem (2.12) Any initial arrangement of pieces is transformable to any final arrangement, using some sequence of piece switches.

Theorem (2.13) A simple case that its initial and final arrangements differ only in a proper tri is solvable.

Theorem (2.14) A simple case that its initial and final arrangements differ only in two succeeding piece switches (not involving the special piece) is solvable.

Algorithm A This algorithms moves the special piece to transform an initial arrangement $\mathbf{R}_i$ to a final arrangement in an $m\times n$ checkerboard if possible. Sequence $\mathbf{S}$ contains the moves in order.

Acknowledgment The author wishes to thank Dr. Ebadollah S. Mahmoodian for his constructive review.

The special routes in plane graphs. **Tatiana Panyukova** (South Ural State University, Russian Federation) IC/CT4424/072

Lots of routing problems arise in definite practical situations. Let a plane undirected graph $G = (V, E)$ be the set of items of all manipulator possible trajectories. The problem is constructing of routes satisfying different restrictions. The restrictions can be classified as local and global. For local restrictions the next edge in a route is defined by the conditions set for current vertex or edge. Examples of such restrictions are straightforward paths; a route in which the next edge is defined by the given cycle order on the set of edges incident the current vertex; a route where some edges should be passed in predefined order.

Local restrictions can be represented as system of allowed transitions T_G or as system of forbidden transitions P_G. Let $P_G(v)$ be a partition of set $E_G(v)$ of edges incident to $v \in V$. Than partition system of graph G will be the system of sets $P_G := P_G(v)|v \in V(G)$. Let $p \in P_G(v)$, $e, f \in p$. Trail which does not contain transitions $e \to v \to f$ and $f \to v \to e$ we shall designate as P_G-compatible and these transitions designate as forbidden. There are lots of researches devoted to the algorithms with local restrictions on the edges order.

The example of global restriction is problem of constructing the cover with ordered enclosing. A plane graph G is a model of a cutting plan, and route covering all the edges in this graph defines the motion of a cutting tool. It is necessary that part cut off from a sheet does not claim additional cuttings. Formally this restriction requires the lack of intersection of interior facets for any initial part of the cutting tool route and the set E. It is intended to present algorithms for constructing the compatible trail-cover of minimal cardinality for an arbitrary connected graph, an algorithm for constructing an ordered enclosing cover, and software for performing these tasks.

A parallel distributed distance-2 graph-coloring algorithm. **Radu Serban** (Lawrence Livermore National Laboratory, USA), Ned Nedialkov (McMaster University, Canada) IC/CT4481/072

We present a parallel, distance-2, bipartite graph coloring algorithm for distributed memory computers. This work is motivated by the need for scalable parallel difference-quotient approximations for ODE/DAE Jacobian matrices for use with sparse direct linear solvers within implicit integrators, such as those in SUNDIALS (Suite of Nonlinear and Differential/Algebraic Equation Solvers).

Although general-purpose, the proposed method takes advantage of (but is also constrained by) its intended use for Jacobian approximations for implicit integration. Based on independent-set coloring of the vertices in the MPI communication layer, combined with one of several sequential coloring methods (such as greedy, incidence degree, saturation degree, etc.), our algorithm has the following features: (a) it colors only the V_2 vertices in the bipartite graph $G = (V_1, V_2, E)$, enough for Jacobian approximation purposes; (b) it does not require information which is hard and/or expensive to obtain (e.g. global distance-1 neighbor information); and (c) it uses the MPI communication pattern imposed by the parallel evaluation of the ODE/DAE user-provided function.

The proposed approach was tested on matrices from the University of Florida Sparse Matrix Collection, as well as on several graphs corresponding to Jacobians of semi-discretized large-scale PDEs.

On the line degree splitting graph of the complete bipartite graphs and complete graphs. **B Basavanagoud** (Karnatak University, Dharwad, India) IC/CT1123/072

In this paper,we introduce the concept of the line degree splitting graph of a graph. Also we present the characterization of line degree splitting graphs for complete bipartite graphs. Further we obtain the results of the characterization of the line degree splitting graphs for complete graphs.

IC/CTS4897/07: Networks, graphs.

Organiser: Dietmar Dorninger (TU Wien, Austria)

On characteristic polynomials of vertex- and edge-weighted molecular graphs. **Dietmar Dorninger** (TU Wien, Austria) IC/CT576/072

We consider molecular graphs whose vertices and edges are weighted by real numbers corresponding to Coulomb and resonance integrals of the underlying chemical compounds. Given a molecular graph G we derive recursive procedures to find the characteristic polynomials of graphs that are obtained from G when new vertices and edges carrying new weights are added to G or vertices and edges of G are substituted. Exploiting these recursions in case G is a cycle or path, we obtain explicit formulas for the characteristic polynomials of the compounds that arise this way and recursive formulas for compounds that have several cycles. Since the zeros of the characteristic polynomials approximately correspond to the energy values of electrons it is of interest to understand the influence of atoms that are added to a given compound or which substitute other atoms. To this end, we look for factors of the characteristic polynomials that do not depend on the weights of the newly introduced atoms and their bonds. In special cases this leads to the investigation of common divisors of Chebyshev polynomials of the first and second kind.

(Work done in collaboration with H. Länger)

On the generalized combinatorial optimization problems and their applications. **Petrica Claudiu Pop** (North University of Baia Mare, Romania) IC/CT1647/072

Classical combinatorial optimization problems can be generalized in a natural way by considering a related problem relative to a given partition of the nodes of the graph into node sets (clusters). We will present some of the most important generalized combinatorial optimization problems: the generalized minimum spanning tree problem, the generalized traveling salesman problem and the generalized assignment problem. We will describe complexity aspects, approximation results, several models based on integer programming and mixed integer programming and some techniques used for getting optimal solutions or sub-optimal solutions for these NP-hard problems. As well we will present some interesting applications of the considered combinatorial optimization problems in network design, location problems, telecommunications, energy distribution, agricultural irrigation, agent service brokering problem, etc.

On digraph strong-searching problems. **Boting Yang** (University of Regina, Canada) IC/CT3230/072

Many real-world problems can be naturally modeled by graph/digraph searching problems. Examples include: capturing intruders in a building or a road system, clearing a complex system of interconnected pipes which is contaminated by some noxious gas, and killing a computer virus in a network system. A graph/digraph searching problem is to find the minimum number of searchers required to capture the intruder hiding in the graph/digraph. In some applications, searchers may not obey the edge directions. For example, if an intruder hiding in a building with one-way locking doors (people can go out but cannot go in without a key), then the intruder must go one-way through a door (suppose that he has no keys), but the security personnel can go both ways through a door because they have the keys. This motivates us to introduce two search models on digraphs: the strong searching model and the mixed strong searching model, in which the intruder must follow the edge directions when they move along edges, but each searcher can move from tail to head or from head to tail along edges. Monotonicity is a very important issue in graph/digraph searching problems. A search strategy is monotonic if once an edge has been cleared, the intruder cannot access to this edge in the rest of the searching process. We prove the monotonicity of both searching models. This implies that in both searching models, the intruder can be captured in a linear number of steps. We show that both searching problems are NP-complete. (This work is done in collaboration with Yi Cao).

A precinct version of the Cops and Robber *game played on powers of graphs.* **Nancy Clarke** (Acadia University, Canada) IC/CT2030/072

The game of *Cops and Robber* is a pursuit game played on a reflexive graph. The cops choose vertices to occupy, and then the robber chooses a vertex. The two sides move alternately, where a move is to slide along an edge or along a loop, i.e. pass. Both sides have perfect information, and the cops win if any of the cops and the robber occupy the same vertex at the same time, after a finite number of moves. The minimum number of cops that suffice to guarantee a win on a graph G is the *copnumber* of G. The game has been considered on infinite graphs but, in this talk, we only consider finite graphs.

We consider the Cops and Robber game when the cops are restricted to moving on assigned "beats" or subgraphs, and bound the copnumbers of powers of graphs under a variety of products. In many cases, the results are shown to be asymptotically exact.

An efficient algorithm for computing permanental polynomials of graphs. **Yan Huo** (Tsinghua University, PR China) IC/CT674/072

An efficient numerical method for computing permanental polynomials of graphs is proposed. It adapts multi-entry expansion of FFT, and is parallel in nature. It is applied to fullerene-type graphs, and works for C56, while the largest fullerene computed before is C40. Extensive numerical computations show that the algorithm is fast and stable.

The work was done in collaboration with Heng Liang and Fengshan Bai.

Graph theory and applications. **Shariefuddin Pirzada** (University of Kashmir, India) IC/CT4141/072

Mathematicians are becoming increasingly aware of the significance of graph theory as it is applied to other areas of science and being widely used to solve various real-world problems. Graph theory is used in organic chemistry, solid-state physics and statistical mechanics, electrical engineering (communication networks and coding theory), computer science (algorithms and computation), optimization theory and operations research. The wide scope of these and other applications has been well-documented cf. [7, 12]. The powerful combinatorial methods found in graph theory have also been used to prove fundamental results in a variety of areas of pure mathematics. My talk, besides giving a general outlook of these facts, will include new graph theoretical proofs of FermatŠs Little theorem and the Nielson-Schreier theorem. New applications to DNA sequencing using minimum vertex covers in graphs (the SNP assembly problem) and scheduling using edge colorings and matchings in graphs (the Timetabling problem) will also be presented.

07: Discrete Mathematics, Posters

IC/PP1127/007: **On chainos ctree graph of a graph.**

Presenter: Sangeeta Bhat (KJ Somaiya College of Arts and Commerce, Mumbai, India)

In this paper, the concept of chainos ctree graph of a graph is introduced. We present the characterization of those graphs whose chainos ctree graphs are noneulerian, hamiltonian, planar, oterplanar, minimally nonouterplanar and maximal outerplanar. also, the necessary and sufficient condition for chainos ctree graphs to have crossing number one or two are established.

IC/PP2009/015: **A way to find optimal persuadable voters in a voting system.**

Presenter: Josep Freixas (Universitat Politècnica de Catalunya, Spain)
Co-author: Montserrat Pons (Universitat Politècnica de Catalunya, Spain)

Let's suppose that certain committee is going to decide, using some fixed voting rules, either to accept or to reject a proposal that affects your interests. From your perception about each voter's position, you can make an *a priori* estimation of the probability of the proposal being accepted. Wishing to increase this probability of acceptance before the votes are cast, assume further that you are able to convince (at least) one voter to improve his/her perception in favor of the proposal.

The question is: which voters should be persuaded in order to get the highest possible increase in the probability of acceptance? In other words, which are the optimal persuadable voters? To answer this question a measure of power is considered, which is useful to identify optimal persuadable voters. Three preorderings in the set of voters, based on the voting rules, are defined and they are used for finding optimal persuadable voters, even in the case that only a qualitative ranking of each voter's inclination for the proposal has been made.

The results we present allow finding optimal persuadable voters for any given simple game and for any possible distribution of voters' preferences in relation with the proposal at hand. The key idea is the introduction of three preorderings in the set of voters.

IC/PP1405/072: **A ranking for the nodes of directed graphs based on game theory.**

Presenter: Jose Miguel Gimenez (Universitat Politècnica de Catalunya, Spain)
Co-author: Rafel Amer (Universitat Politècnica de Catalunya, Spain)
Co-author: Antonio Magana (Universitat Politècnica de Catalunya, Spain)

A cooperative game is a pair (N, v), where N is a finite set of agents or players and v is the so-called characteristic function, which assigns to every group of players or coalition S a real number $v(S)$, the worth or utility that the coalition S can obtain in the situation described by the game.

A central problem of Game Theory consists of distributing the total utility by using acceptable allocation rules. The most important solution concept for cooperative games is the Shapley value, whose payoff to each player is a weighted sum of his/her marginal contributions to the coalitions. This solution verifies symmetry and efficiency –the sum of payoffs to all players agrees with the utility of N–.

In a classical cooperative game, every coalition can form. Nevertheless, a directed graph on N can model the feasible coalitions according to the sequences of nodes obtaineed by means of its oriented edges. The cooperation is only possible when the players are related by means of the directed graph. This idea directly leads to our solution concept for a game modified by a directed graph: cooperation is possible when there exists accessibility.

The introduced solution for games modified by directed graphs is an extension of the Shapley value. If a game is symmetric –the utilities only depend on the coalition size–, the Shapley value assigns a same payoff to all players. Thus, according to our introduced solution, the allocations to the players in a symmetric game only depend on the geometry imposed by the directed edges.

Each oriented network can be described by means of a directed graph. For obtaining a ranking among the nodes without a predefined game, we use a family of cooperative games: the test games. It is an exogenous procedure with respect to the oriented network. The test games are chosen among a particular type of games with the condition of symmetry.

08: Probability and Statistics, Minisymposia

IC/MP151/008: **Statistical methods in inverse problems.**

Organiser: Thorsten Hohage (Universität Göttingen, Germany)
Co-organiser: Hanna Pikkarainen (RICAM Linz, Austria)

In inverse problems, one looks for causes for a desired or observed effect. Inverse problems are usually ill-posed in the sense that the solution depends very sensitively on data noise. Therefore, regularization strategies and the study of the dependence of approximate solutions on the noise are essential issues.

Topics discussed in this minisymposium include nonlinear statistical inverse problem, choice of regularization parameters based on multi-resolution analysis, Bayesian approaches, and convergence rate analysis from a Bayesian perspective with applications to astronomy and mass spectroscopy.

Convergence rates for the Bayesian approach to linear inverse problems. **Hanna Pikkarainen** (RICAM Linz, Austria) IC/MT2657/008

Recently, the metrics of Ky Fan and Prokhorov were introduced as a tool for studying convergence in stochastic ill-posed problems. In this work, we show that the Bayesian approach to linear inverse problems can be examined in the new framework as well. We consider the finite-dimensional case where the measurements are disturbed by an additive normal noise and the prior distribution is normal. Convergence and convergence rate results are obtained when the covariance matrices are proportional to the identity matrix.

The work has been done in collaboration with Andreas Hofinger, Johann Radon Institute for Computational and Applied Mathematics, Austrian Academy of Sciences and has been supported by the Austrian National Science Foundation FWF through the project SFB F1308.

Measurements and infinite-dimensional statistical inverse theory. **Sari Lasanen** (Oulun Yliopisto, Finland) IC/MT2268/008

The most important ingredient in the statistical inverse theory is the indirect and noisy measurement of the unknown. Without the measurement, the formula for the posterior distribution becomes useless. However, insertion of the measurement to the posterior distribution is not always simple. Especially this happens when the measurement and the unknown are infinite-dimensional.

In the general setting, the posterior distribution is defined as a regular conditional probability. Hence it is known up to almost all measurements which is inconvenient when we are given a single measurement. This shortage is covered in the finite-dimensional statistical inverse theory by fixing versions of probability density functions. A usual choice is to consider continuous probability density functions. Unfortunately, infinite-dimensional probability measures lack density functions which prohibits us from using the same method in the general setting. In this presentation, other possibilities for fixing the posterior distributions are discussed, especially in the Gaussian framework.

Multi-scale selection of the stopping criterion for MLEM reconstructions in PET. **Nicolai Bissantz** (Ruhr-Universität Bochum, Germany), Axel Munk (Universität Göttingen, Germany), A Mair (University of Florida, USA) IC/MT1007/008

In this paper we present a fully data-driven selection algorithm for the stopping criterion for MLEM reconstructions in PET. The method can be generalized to various other reconstruction algorithms, and is based on a statistical analysis of the residuals between projected model and data.

To this end we test whether the residuals are consistent with the hypothesis of being solely due to Poisson noise. Moreover, our method includes a multiresolution approach, i.e. we test whether the residuals are consistent with pure Poisson noise for all possible re-binning of the data into increasing bin sizes in the detector space, and at all positions.

Technically, our method is based on the almost sure limiting behaviour of partial sums of the residuals. We determine the rate function which appears in the corresponding almost sure limit theorem for Poisson noise, and which is different from the Gaussian noise case. Finally, we present results from a Monte Carlo study which demonstrates the performance of the method.

On statistical linear inverse problems and multiresolution schemes. **Monika Meise** (Universität Duisburg-Essen, Germany) IC/MT1716/008

A multiresolution analysis of the residuals of an approximating function provides a criterion to decide whether an approximation is sufficiently close to the data or not. Using the model

$$y_i = Kf(t_i) + \varepsilon_i \qquad i = 1, \dots, n$$

where K is a linear operator and ε_i i.i.d. $\mathcal{N}(0, \sigma^2)$ it is shown how the idea can be combined with various forms of regularization to provide an adequate approximating function. One example is the minimization of the total variation which results in a function f_n with a small number of extreme values such that Kf_n gives a good approximation to the data.

IC/MP577/008: **Probabilistic numerical methods for PDEs and stochastic PDEs.**

Organiser: Wesley Petersen (ETH Zürich, Switzerland)
Co-organiser: Michael Mascagni (Florida State University, USA)

Monte Carlo methods for transport problems, turbulence, and high dimensional PDEs usually involve numerically solving a stochastic differential equation,

$$dX = b(X)dt + \sigma(X)dW(t),$$

where W is a vector of Wiener processes. Coefficients $b(X)$ and $\sigma(X)$ are the drift vector and square root of the diffusion matrix respectively; these appear in the PDE. Functionals of this process X will involve source terms and potentials, even non-linear variants. These talks will explore stochastic numerical methods for the solutions of PDEs. By enlarging the vector space for X, discretized versions of SPDEs can be similarly treated. Models for turbulence and financial systems can often be formulated in this way.

p-Sparse BEM for weakly singular integral equation with random data. **Alexey Chernov** (ETH Zürich, Switzerland), Christoph Schwab (ETH Zürich, Switzerland) IC/MT4992/008

We consider the weakly singular boundary integral equation $\mathcal{V}u = g$ on a randomly perturbed smooth closed surface $\Gamma(\omega)$ with deterministic g or on a deterministic closed surface Γ with stochastic $g(\omega)$. The aim is the computation of the moments $\mathcal{M}^k u := \mathbb{E}[\otimes_{i=1}^k u]$, $k \geq 1$, if the corresponding moments of the perturbation are known. The problem on the stochastic surface is reduced to a problem on the nominal deterministic surface Γ with the random perturbation parameter $\kappa(\omega)$. Note, that $u(\omega)$ depends nonlinearly on $\kappa(\omega)$.

Resulting formulation for the kth moment is posed in the tensor product Sobolev spaces and involve the k-fold tensor product operators $\mathcal{V}^{(k)} = \otimes_{i=1}^k \mathcal{V}$. The standard full tensor product Galerkin BEM requires $\mathcal{O}(N^k)$ unknowns for the kth moment problem, where N is the number of unknowns needed to discretize the nominal surface Γ. Based on [3], we develop the p-sparse grid Galerkin BEM to reduce the number of unknowns to $\mathcal{O}(N(\log N)^{k-1})$ (cf. [1], [2] for the wavelet approach).

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A finite-element method for dilute polymers: numerical experiments and theoretical results. **Marco Picasso** (École Polytechnique Fédérale de Lausanne, Switzerland), Andrea Bonito (Univ. Maryland at College Park, USA), Philippe Clément (Universiteit Leiden, The Netherlands) IC/MT3534/008

A finite element method for solving viscoelastic flows (more precisely dilute polymer solutions) with complex free surfaces is presented. The method applies to macroscopic (deterministic) models such as Oldroyd-B, but also to mesoscopic (stochastic) models such as FENE dumbbells. Numerical results will be presented for complex free surface flows such as jet buckling or filament stretching.

Finally, existence and convergence of a stochastic finite element method will be presented for a simplifed Hookean dumbbells problem.

FE calculation of the 2-point correlation of the solution of an elliptic SPDE. **Bastian Pentenrieder** (ETH Zürich, Switzerland) IC/MT4991/008

Let (Ω, Σ, P) be a probability space. We consider the Poisson equation $-\triangle u = f$ in a domain D with Dirichlet boundary conditions and stochastic right hand side $f \in L^2(\Omega, \mathrm{d}P; H^{-1}(D))$. The aim is to determine the two-point correlation of the solution, $C_u(x,y) := \int_\Omega u(x,\omega)\, u(y,\omega) \mathrm{d}P(\omega)$, from the two-point correlation C_f of the stochastic loading.

C_f is assumed to belong to particular Sobolev spaces that are weighted w.r.t. the diagonal of the product domain $D \times D$, thus allowing to model singular behavior. For the solution of the problem, we employ an hp-FEM discretization resolving possible singularities on the diagonal. Numerical experiments will be presented showing exponential convergence w.r.t. the maximum polynomial degree.

This is joint work with Prof. Christoph Schwab.

IC/MP19/010: Environmental economics and stochastics.

Organiser: Pauline Barrieu (London School of Economics, UK)

With the increased awareness of global warming issues, biodiversity preservation and, more generally, of the notion of ecology, environmental economics has become a growing field of research.

More and more sophisticated techniques and methods, from probability in particular, are used and developed to study these questions, following partially the approach already adopted in mathematical finance some decades ago.

The focus of this mini-symposium session will be put on the use of both probabilistic and financial techniques in the study of environmental issues, such as stochastic optimal control, real option analysis, general equilibrium theory, or some particular forms of Backward Stochastic Differential Equations. The emphasis will be in particular on how these tools can help solving environmental problems and improving the overall management of the Environment.

Different topics will be presented in this mini-symposium session. They have however in common the study of the decision taking process, either using real option theory and applying it to some specific problems such as biodiversity and species protection (A. Leroux and P. Lasserre) or choice of decontamination policies (B. Sinclair-Desgagn), or an equilibrium approach for the hedging of some climate risk using contingent securities (U. Horst).

A real options approach to forest management and the protection of caribous from extinction. **Pierre Lasserre** (Université du Québec a Montréal, Canada) IC/MT1369/010

Uncertainty is a dominant feature of forestry and wildlife-management decision making. Aggravating this challenge is the irreversibility of some decisions, resulting in the loss of economic opportunities or the extinction of wildlife populations. We adapt the Real Options approach to determine the optimal time wood harvesting should be interrupted and banned in a forest used as habitat by some valuable animal species. The model is applied to the case of the woodland caribou (*Rangifer tarandus caribou*). Habitat growth is a mean-reverting stochastic process and it is believed by biologists that the caribou herd will become extinct if its habitat diminishes enough to reach some threshold value. While banning timber harvesting does not guarantee that the caribou habitat will be prevented from reaching the extinction threshold, it will reduce the probability of that event thereby increasing the probability of caribou survival. However there is a cost in banning timber harvesting and the decision to do so must optimally trade that cost against the probability of survival. The model incorporates economic, ecological and social features present in forest management decision making. The model is calibrated by applying a Monte Carlo approach based on forest data from Eastern Labrador, Canada.

A real options approach to brownfields and polluted-sites remediation. **Bernard Sinclair-Desgagné** (HEC Montreal, Canada) IC/MT1742/010

We consider the matter of managing the remediation of a particular polluted site. The contamination level of this site evolves randomly over time (with a drift) and can be represented as a stochastic process. Within a certain time horizon T, this level should reach a threshold L set by the regulator, or the manager will incur a significant fine F. The manager now contemplates two feasible remediation technologies: a flexible, cheap but uncertain one (natural remediation, say), and an irreversible, expensive but certain one (excavation and incineration, say). Using the machinery of real options, we first characterize and compute the manager's optimal strategy. Under this strategy, the manager starts with using the flexible technology and switches to the irreversible treatment if contamination remains above some (endogenous level) K after a certain (endogenous as well) time t.

Real options in biodiversity conservation. **Anke Leroux** (La Trobe University, Australia) IC/MT3994/010

The irreversible conversion of forests matters for biodiversity conservation in view of exogenous and endogenous types of risk. Natural ecological variations give rise to the former risk whereas the latter encompasses the consequences of extinction debt, which is a function of the rate of land conversion. Optimal dynamic land allocation decisions are derived numerically within a real options framework, where the value of biodiversity follows a controlled diffusion process. Economic-ecological system dynamics are analysed in the conservation and conversion zones for Costa Rica. It is found that extinction debt results in two competing forces with the mean effect increasing optimal biodiversity conservation, whereas the variance effect leads to greater conversion of land. The costs of extinction debt under optimal and non-optimal policy designs are quantified.

On the spanning property of risk bonds priced by equilibrium. **Ulrich Horst** (University of British Columbia, Canada) IC/MT611/010

We propose a method of pricing financial securities written on non-tradable underlyings such as temperature or precipitation levels. To this end, we analyze a financial market where agents are exposed to financial and non-financial risk factors. The agents hedge their financial risk in the stock market and trade a risk bond issued by an insurance company. From the issuer's point of view the bond's primary purpose is to shift insurance risks related to non-catastrophic weather events to financial markets. As such its terminal payoff and yield curve depend on an underlying climate or temperature process whose dynamics is independent of the randomness driving stock prices. We prove that if the bond's payoff function is monotone in the external risk process, it can be priced by an equilibrium approach. The equilibrium market price of climate risk and the equilibrium price process are characterized as solution of nonlinear backward stochastic differential equations. Transferring the BSDEs into PDEs, we represent the bond prices as smooth functions of the underlying risk factors.

IC/MP278/010: Applications of random matrices to physics and engineering.

Organiser: Ioana Dumitriu (University of Washington, USA)
Co-organiser: Alan Edelman (Massachusetts Institute of Technology, USA)

Random matrix theory is an area that brings together a large number of fields, from "classical" quantum physics and multivariate statistics, to "modern" wireless communications, computational biology, and numerical analysis, and to "exotic" number theory.

Though random matrix theory has been around since the late 1920s, it is in the last two decades that the number of applications has seen tremendous growth. Today, random matrix distributions have been connected to a wide variety of problems, from noise modeling in multiple-input, multiple-output channels, to the study of traffic patterns on German highways.

In addition to the availability of a large body of theory, this growth is also due to the recent increases in computational speed and memory, which have made it possible for software tools to be built and for distributions to be computed either empirically, with the help of matrix models, or theoretically, through special functions and advanced mathematical techniques. Via fast algorithms and mathematical tricks, computations that used to take days are now reduced to seconds, and, for the first time, made practical.

Our mini-symposium would consist of 3–4 presentations by top researchers who apply methods and tools from random matrix theory to the study of problems from signal processing, wireless communications, and statistical physics. Bringing together such a group of people would stimulate interest interest in random matrix theory, build new connections between fields, and spread information about the important open problems that random matrix theory might be able to provide an answer for.

Random matrices: a brief survey of theory and applications . **Ioana Dumitriu** (University of Washington, USA) IC/MT3522/010

How many fields of mathematics, physics, and engineering which make use of random matrix theory can one name?

The magnitude of the answer might surprise you. From the Riemann ζ-function to random permutations and from particle interactions in heavy nuclei to the capacity of MIMO channels, random-matrix distributions are being successfully used for modeling and/or explaining natural and technological phenomena. This talk will survey some of the fields where random matrix theory makes an impact, and discuss some of the theoretical distributions and models that are of interest.

The role of random matrices in compressed sensing. **Emmanuel Candès** (California Institute of Technology, USA) IC/MT3710/010

In the last few years, a new sampling or sensing theory has emerged which goes somewhat against the conventional wisdom and common practice in signal or image acquisition. This theory claims that it is possible to recover signals and images faithfully from what appear to be highly incomplete sets of data, i.e. from far fewer data bits than traditional methods use. This theory relies on two fundamental premises: 1) sparsity or compressibility of the object we wish to recover and 2) incoherence between the domain in which the object is sparse and that in which it is acquired.

It turns out that a convenient way to design incoherent measurements is by nonadaptive random sensing, hence the key role played by random matrices. Specifically, we wish to find matrices for which sparse vectors are 'away' from the (large) null space of the matrix or more quantitatively, which act on sparse vectors as near isometries—a property sometimes referred to as a uniform uncertainty principle in the literature. The talk will discuss the importance of this property together with some key results in compressed sensing, and show how to design random properties obeying this principle; e.g. by either randomly drawing the entries independently at random or by selecting the rows of a fixed orthogonal transformation uniformly at random. We will also show how certain special random matrices can be used effectively to speed up the computations required to recover the signal of interest from undersampled data.

β ensembles and simple scale-free graphs. **Petr Seba** (Czech Academy of Sciences, Czech Republic) IC/MT3751/010

We show that the eigenvalues of a simple quantum graph display spectral statistics that is well described by a beta ensemble. Depending on the topology of the graph one can obtain ensembles with beta<1 as well as with beta>1.

Recent results on the eigenvalues of random matrices with application to wireless communication systems. **Moe Win** (Massachusetts Institute of Technology, USA), Marco Chiani (Università di Bologna, Italy), Alberto Zanella (Consiglio Nazionale delle Ricerche, Italy) IC/MT5036/010

The increasing demand for wireless communications has generated interest in multiple antenna systems and, more recently, in multiple-input-multiple-output (MIMO) systems. Such systems can provide great advantages due to the presence of multiple rays propagation, causing the elements of the channel gain matrix to flutuate. Such channel gain matrix can be well modelled by random matrix with appropriate distribution. In particular, performance of MIMO systems depends on the distribution of the eigenvalues of hermitian matrices, whose dimensions are related to the number of transmitting and receiving antenna elements. In several practical situations, the elements of the channel matrix can be modeled as complex Gaussian random variables; this is the case, for example, when the propagation environment is characterized by Rayleigh or Rician fading. Under these conditions, the performance of the wireless communication systems is related to the distribution of the eigenvalues of Wishart matrices or general quadratic forms. In this talk, we describe the main problems in MIMO wireless communication, showing the relation with the theory of random matrices. More specifically, we present recent results on the distribution of the eigenvalues of Wishart matrices and related quadratic forms, and discuss the implications in terms of the performance of wireless communications.

IC/MP345/010: Monte-Carlo methods with spatially-structured randomness.

Organiser: Peter Kramer (Rensselaer Polytechnic Institute, USA)
Co-organiser: Karl Sabelfeld (Weierstraß-Institut Berlin, Germany)

The speakers in this session will describe recent research on computational techniques for representing and simulating physical processes in which some spatially distributed fields cannot be described precisely due to insufficient data. Due to the physical interactions between different regions, the uncertainty must generally be assumed to have spatial structure and is therefore typically modeled by a random field with a nontrivial spatial correlation structure. The talks in this session will describe several ways of representing the spatially structured random field in a computationally efficient way, and discuss applications such as simulating a flow through a porous medium with unresolved pore structure.

Comparative analysis of multiscale Gaussian random-field simulation algorithms. **Peter Kramer** (Rensselaer Polytechnic Institute, USA), Orazgeldi Kurbanmuradov (Turkmenian State University, Turkemistan), Karl Sabelfeld (Weierstraß-Institut Berlin, Germany) IC/MT3178/010

We analyze and compare the efficiency and accuracy of the Fourier-Wavelet and Randomization Methods for homogeneous random fields with multiscale resolution. Such random fields arise in numerical simulations and models for porous media and turbulent flows, as well as other disordered media. We focus on fractal Gaussian random fields with Kolmogorov-type spectra. We provide some conceptual and numerical comparison of the various cost contributions to each random field simulation method (overhead, cost per realization, cost per evaluation).

We find that when evaluating ensemble averaged quantities like the correlation and structure functions, as well as some multi-point statistical characteristics, the Randomization method can provide good accuracy with less cost than the Fourier-wavelet method. The cost of the Randomization method relative to the Fourier-wavelet method, however, appears to increase with the complexity of the random field statisics which are to be calculated accurately. Moreover, the Fourier-wavelet method has better ergodic properties, and hence becomes more efficient for the computation of spatial (rather than ensemble) averages which may be important in simulating the solutions to partial differential equations with random field coefficients.

Memory effects and ergodicity for diffusion in spatially-correlated velocity fields. **Nicolae Suciu** (Friedrich-Alexander University Erlangen-Nürnberg„ Germany), Karl Sabelfeld (Weierstraß-Institut Berlin, Germany), Calin Vamos (T. Popoviciu Institute, Romania), Constantin Andronache (Boston College, USA) IC/MT2851/010

Diffusion in space variable velocity fields shows a typical memory effect produced by correlations between initial conditions and velocity fluctuations on trajectories. Such correlations cause supplementary "memory terms" of the dispersion (mean square displacement of diffusing particles). We demonstrate that by theoretical investigations based on Itô and Fokker-Planck equations and numerical simulations as well. Strictly specking, only Fickian diffusion is free-of-memory. Nevertheless, for statistically homogeneous random fields, the ensemble average of the velocity correlation on trajectories yields a memory-free dispersion which does not depend on initial conditions. This quantity describes the enhancement of diffusion in a variety of models for transport in turbulent atmosphere, ionized plasma, or porous media. The reliability of the model for single replicates of the physical system requires some "ergodic behavior" in a large sense. We investigated this eventuality by root mean square deviations of actual dispersion from memory-free dispersion. The so defined "ergodicity range" was found to be strongly dependent on initial conditions. The increase of the ergodicity range for large supports of the initial concentration is essentially caused by memory terms. Moreover, the larger the anisotropy of the initial concentration is, the larger the memory terms of dispersion in the anisotropy direction are. This relation could be used in practice to identify the source of contamination from available measurement data.

IC/MP351/010: Stochastic modeling in microbiology and microphysics.

Organiser: Peter Kramer (Rensselaer Polytechnic Institute, USA)

The speakers in this session will describe applications of the methods of stochastic processes and nonequilibrium statistical mechanics toward the modeling and simulation of microphysical processes, particularly those occuring within biological cells. Several of the talks will explore the framework of molecular motors from mathematical, biological, and physical perspectives.

Effective transport properties for flashing ratchets using homogenization theory. **Juan Latorre** (Rensselaer Polytechnic Institute, USA), Peter Kramer (Rensselaer Polytechnic Institute, USA), Grigorios Pavliotis (Imperial College London, UK) IC/MT4270/010

We investigate the transport properties of Brownian flashing ratchet motors, which model molecular motors moving on periodic structures and extract useful work from the unbiased thermal environment by keeping them away from thermodynamic equilibrium. The approach for modeling these motors is set in the context of Brownian motors, since the interactions of the motor with the aqueous environment must be taken into account. For enzymes such as kinesin, the strength of thermal and damping forcing overtake the inertial terms, thus the dynamics of the motor are reduced to an overdamped equation. The interactions of the motor with the thermal environment are incorporated in the system through additive white noise, while the external driving is modeled as a multiplicative stochastic noise. We use homogenization theory to develop rigorous computations for the long time limit features of the motor, given by the effective drift and diffusivity, which may be calculated by solving cell problems (homogenized equations.) We analyze the dependence of the transport properties with respect to the parameters of the system and, ultimately, the efficiency of the motor, characterized by the Peclét number. For the case in which the motor is driven by a piecewise periodic linear potential and the system is kept far from equilibrium through a discrete state multiplicative Markov chain, we are able to solve the cell problem analytically up to a set of constants. When the external multiplicative noise is replaced by Gaussian noise, we study the solution of the cell problem both asymptotically and numerically. We compare our analytic findings and numerical solutions of the homogenized equations with Monte Carlo simulations.

Motor potential profile and a method for reconstructing it from data. **Hongyun Wang** (UC Santa Cruz, USA) IC/MT3716/010

We study molecular motors in the framework of coupled Fokker-Planck equations. The motor's motion is modeled explicitly as a stochastic continuous motion driven by a potential that changes with the chemical occupancy state. Therefore, the motor operation is specified by a set of potentials, each corresponding to one chemical occupancy state, and by the transition rates among these states. Based on the current experimental data, it is still unrealistic to determine all these potentials and transition rates. Here we propose a single potential by averaging over all chemical states and use it to characterize the motor operation. The most important advantage of working with this single potential is that it can be reconstructed from measured time series of motor positions in single molecule experiments.

Chiral separation in microflows. **Marcin Kostur** (Universität Augsburg, Germany) IC/MT3300/010

Molecules that only differ by their chirality, so called enantiomers, often possess different properties with respect to their biological function. Therefore, the separation of enantiomers presents a prominent challenge in molecular biology and belongs to the "Holy Grail" of organic chemistry. In this talk a new separation technique for chiral molecules that is based on the transport properties in a microfluidic flow with spatially variable vorticity will be presented. Because of their size the thermal fluctuating motion of the molecules must be taken into account. These fluctuations play a decisive role in the proposed separation mechanism.

Fusion versus endocytosis: the stochastic entry of enveloped viruses. **Tom Chou** (UC Los Angeles, USA) IC/MT3199/010

Viral infection requires the binding of receptors on the target cell membrane to glycoproteins, or *spikes*, on the virus membrane. Fusion peptides that make up part of these spikes on the viral membrane may then be triggered by pH changes or binding of additional coreceptors. Thus, binding of virus envelope proteins to cell surface receptors not only initiates the viral adhesion and the wrapping process necessary for internalization, but also starts the direct fusion process. Both fusion and internalization may be viable pathways for some viruses, under appropriate conditions. We develop a stochastic model for viral entry that incorporates both receptor mediated fusion and endocytosis. The relative probabilities of fusion and endocytosis of a virus particle initially nonspecifically adsorbed on the host cell membrane are computed as functions of receptor concentration, binding strength, and number of spikes. We find the parameter regimes where each pathway is expected to arise and discuss possible experimental tuning of these parameters.

IC/MP352/010: Effective stochastic modeling of multiscale systems.

Organiser: Peter Kramer (Rensselaer Polytechnic Institute, USA)

The speakers in this session will describe recent research on a variety of approaches toward representing high dimensional dynamical systems with a wide range of time scales in terms of reduced effective equations with stochastic terms. The talks will discuss both mathematical aspects of these procedures and the means by which the coefficients of the reduced equations can be computed numerically in practice.

Parameter estimation for multiscale diffusions. **Andrew Stuart** (University of Warwick, UK) IC/MT1535/010

I will describe recent work aimed at the problem of identifying effective homogenized or averaged diffusions (SDEs) from multiscale time series data.

Diffusive transport in periodic structures: underdamped dynamics. **Grigorios Pavliotis** (Imperial College London, UK) IC/MT3764/010

We study the Langevin dynamics of a Hamiltonian system with periodic potential which is subject to dissipation and is forced by white noise. We are interested in analyzing the long time asymptotics of this system as a function of the friction coefficient γ at a fixed temperature T. It is well known that under the standard diffusive rescaling the particle position converges in distribution to a Brownian motion with covariance matrix D. We study the dependence of D on γ, in particular for $\gamma \ll 1$. Furthermore we show that under an appropriate space–time rescaling, the particle position converges in distribution to a Brownian motion in the limit as $\gamma \to 0$.

Time-series analysis in multiple dimensions: dimension reduction, model fitting and prediction. **Illia Horenko** (Freie Universität Berlin, Germany) IC/MT1536/010

Due to the development of computational and measuring facilities in biology and in geo-sciences, large amounts of measured and simulated information from all kinds of processes were accumulated. All of these complex processes share the following properties:

- they are multi-dimensional, i. e. they can be completely described and understood only from the observation or measurement of many of their characteristics simultaneously,
- the dynamics of the system is typically non-linear and non-equilibrium,
- many complex systems exhibit (hidden) phases or regimes which are persistent over the long periods of time but are not (asymptotically) stable.

Several newly developed *data-based methods* for simultaneous dimension reduction, clustering and fitting of the SDE models for the analyzed multidimensional data will be presented and illustrated with some examples from molecular dynamics, climate and finance.

Stochastic modelling of spatially-distributed systems. **Radek Erban** (University of Oxford, UK) IC/MT3631/010

Many cellular and subcellular biological processes can be described in terms of diffusing and chemically reacting species (e.g. enzymes). Such reaction-diffusion processes can be mathematically modelled using either deterministic partial differential equations or stochastic simulation algorithms. The latter provide a more detailed and precise picture, and several stochastic simulation algorithms have been proposed in recent years. Such models typically give the same description of the reaction-diffusion processes far from the boundary of the simulated domain, but the behaviour close to a reactive boundary (e.g. a membrane with receptors) is model-dependent. In this talk, we show the correct choice of the boundary conditions for different stochastic models. We also show how approximate macroscopic mean-field equations can be used to improve the convergence of equation-free coarse-grained methods for the stochastic spatially distributed systems (e.g. for the stochastic reaction-diffusion processes).

IC/MP351/010: Stochastic modeling in microbiology and microphysics. #2

Organiser: Peter Kramer (Rensselaer Polytechnic Institute, USA)

(For abstract, see session #1 above.)

Collective coordinates and the mechanism for conformational transitions of complex molecules. **Tomohiro Yanao** (Kyoto University, Japan), Wang Koon (California Institute of Technology, USA), Jerrold Marsden (California Institute of Technology, USA), Yannis Kevrekidis (Princeton University, USA) IC/MT3699/010

Conformational transitions of polyatomic molecules, clusters and biopolymers are of great interest in current chemical and biological physics. Since this kind of collective motion involves many internal degrees of freedom coherently, reduction of the dimensionality is crucial for the deep understanding of their mechanisms. In this talk, we will first describe the conformational dynamics of an N-atom molecule by the three gyration radii and the (3N-9) hyperangular variables based on the framework of geometric mechanics and the hyperspherical coordinates. The three gyration radii generally serve as slow collective variables, while the remaining hyperangular variables serve as rapidly oscillating bath modes. The averaged equations of motion for the three gyration radii reveal that these collective variables are subject to two different kinds of competitive forces: One is the ordinary potential force, and the other is a kinematic force called internal centrifugal force. The potential force generally works to keep the mass distribution of the system compact and symmetric, while the internal centrifugal force works to distort and inflate it. Thus the internal centrifugal force critically initiates the large-amplitude conformational transitions of molecules. We will quantify the competition between the potential force and the internal centrifugal force by introducing an effective energy in the three-dimensional space of gyration radii, and explain the structural preference of the system between symmetric and asymmetric conformations. The present method should be useful for the systematic reduction of dimension as well as for the identification of dynamical barriers for a wide class of molecular reactions.

Optimal prediction in classical molecular dynamics. **Carsten Hartmann** (Freie Universität Berlin, Germany) IC/MT1560/010

Computer simulations of dynamical systems are a major tool for understanding certain chemical and biological processes on the molecular level. From a statistical mechanics point of view these molecular processes are responsible for the thermodynamical properties of the system. Hence a crucial point in molecular dynamics is the sound causal explanation of observable macroscopic properties in terms of the dynamics of a single molecule and in terms of dimension-reduced models. This talk addresses model reduction for mechanical molecular models from the viewpoint of projection operator techniques and optimal prediction. Given a suitable reaction coordinate, we derive a simple expression for the optimal prediction Hamiltonian, which is non-separable and contains an effective potential which, surprisingly, is not the standard free energy. The effective Hamiltonian allows for a lucid physical interpretation as a mechanical system with a curved configuration space. We illustrate that optimal prediction performs remarkably well, when it is applied to molecular dynamics problems that are intrinsically non-deterministic (e.g., conformation dynamics). It turns out that the intrinsic geometry of the reaction coordinate can have significant dynamical effects on the conformation dynamics that compete with the effects induced by the potential energy.

Stochastic dynamics of rigid bodies in application to DNA base(-pair) sequences. **John Maddocks** (École Polytechnique Fédérale de Lausanne, Switzerland) IC/MT2326/010

A basic issue for rigid base(-pair) models of DNA is the extraction of a complete set of sequence-dependent energy parameters from MD simulations. Explicit formulas are obtained in terms of equilibrium averages in the statistical mechanics sense. In the talk we consider the construction of (stochastic) dynamical systems of interacting rigid bodies in thermal equilibrium with a heat bath allowing for sampling of the canonical ensemble by means of long-term simulation. The first approach is stochastic Langevin dynamics that can be regarded as a mechanical system with additional friction and noise. As a second model for the interacting body-system we introduce the Smoluchowski equation that is derived from the Langevin

system by considering the friction limit $\gamma \to \infty$. It is restricted to configuration space and is ergodic wrt. the Boltzmann measure scaled by a metric factor going back to the rotational dynamics.

IC/MP352/010: Effective stochastic modeling of multiscale systems. #2

Organiser: Peter Kramer (Rensselaer Polytechnic Institute, USA)

(For abstract, see session #1 above.)

Stochastic mode-reduction in large deterministic systems. **Ilya Timofeyev** (University of Houston, USA) IC/MT3212/010

A new stochastic mode-elimination procedure is introduced for a class of deterministic systems. Under assumptions of mixing and ergodicity, the procedure gives closed-form stochastic models for the slow variables in the limit of infinite separation of time-scales. We show that under these assumptions the ad-hoc modification of the nonlinear self-interactions of the fast degrees of freedom can be avoided. The procedure is applied to the Truncated Burgers-Hopf (TBH) system as a test case where the separation of timescale is only approximate. It is shown that the stochastic models reproduce exactly the statistical behavior of the slow modes in TBH when the fast modes are artificially accelerated to enforce the separation of timescales. It is shown that this operation of acceleration only has a moderate impact on the bulk statistical properties of the slow modes in TBH. As a result, the stochastic models are sound for the original TBH system.

Averaging for diffusive fast–slow systems with metastability in the fast variables. **Jessika Walter** (École Polytechnique Fédérale de Lausanne, Switzerland) IC/MT2328/010

In complex system modeling one often finds mathematical models that consist of many differential equations with different temporal and spatial scales. One of the basic approaches to the complexity reduction is based on elimination of fast degrees of freedom (DOF) from the original equation by averaging according to the equilibrium probability measure corresponding to the exploration of the accessible fast state space. In this talk we consider different scenarios where the system exhibits metastability in the fast variables. To this end, we switch attention to the formal analysis of the associated Fokker-Planck equation in the asymptotic limit $\epsilon \to 0$ of infinitely fast variables, and reconsider the derivation of the effective slow (essential) dynamics over order unity time scale. Separating the time scale over which the slow dynamics proceed and the time scale of the metastable transitions will enable us to obtain a categorization of the various kinds of long-time effective behaviour that can emerge from the original system.

IC/MP180/010: Multiscale models and methods for inference.

Organiser: Sofia Olhede (Imperial College London, UK)

Observed data sets in many areas of application, such as oceanography, climatology, and medical imaging, are often non-stationary. This makes the development of non-stationary stochastic models and inferential procedures very important. Given the local and structured form of many physical processes, methods that treat the data distinctly at given scales, simplify both the modelling and analysis of such data sets. This session will synthesise recent results in the development of statistical multiscale models, inferential methods and their application. Examples of prediction, clustering and estimation methods based on using multiscale techniques will be presented, as well as innovative uses of such methods for given applications, where a physical interpretation of the multiscale structure can be made. Both 1-D and higher dimension data sets will be considered, and the numerical aspects of the implementation will be discussed, as well as analysis methods suitable for irregularly sampled data sets. The session will thus present examples to illustrate the power and flexibility of recently proposed multiscale statistical methods, and will draw together parallel and complimentary innovations, both to connect and highlight existing state of the art methods, but also to encourage future applications and development of theory and methods.

Multiscale methods and sparsity for inference. **Sofia Olhede** (Imperial College London, UK) IC/MT2804/010

Recent advances in the modelling and analysis of structured data have been developed to match the ever more difficult challenges of the 'information age' we currently inhabit. A deluge of data is routine collected in many application areas, such as medical imaging or finance, that is produced by very complicated generating mechanisms. To tackle such problems modern inferential procedures use sparsity and multiscale features of data, and build on highly sophisticated recent advances in optimisation and statistics. The methods formally treat inferential problems such as clustering, prediction and estimation, using the posited structure of the data, to in some cases even resolve problems that were otherwise not tractable.

This talk will provide an overview of new developments in the area of multiscale and sparsity based methods for inference. Methods from compressed sensing, second generation multiscale analysis, and other recently proposed frameworks for treating structured data, will be touched upon. We aim to connect and contrast novel models and methods to those already in the literature, i.e. the evolutionary spectrum and the Cramer representation of a process. We shall discuss results in generality, providing a road map for the session, as well as touch upon successful application areas.

As an example, we shall use a new multiscale multi-variate model corresponding to constraining the replication of structure across the elements of a vector-valued time series. The model allows for the estimation of both shared and individual variable structure, despite being non-stationary. To show the power of such methods we apply them to data sets collected from Oceanography.

This work was done in collaboration with Dr Jonathan Lilly, Earth and Space Resources, Washington, Seattle.

A multiscale approach for statistical characterization of functional images. **Rainer von Sachs** (Université catholique de Louvain, Belgium) IC/MT2621/010

In this paper we use an approach of spatial multiscales for an improved characterization of functional pixel intensities of images. Examples are numerous such as temporal dependence of brain response intensities measured by fMRI or frequency dependence of NMR spectra measured at each pixel. The overall goal is to improve the misclassification rate in clustering (unsupervised learning) of the functional image content into a finite but unknown number of classes. Hereby we adopt a non-parametric point of view to reduce the functional dimensionality of the observed pixel intensities, modelled to be of a very general functional form, by a combination of "aggregation" and truncation techniques. Clustering is applied via an EM-algorithm for estimating a Gaussian mixture model in the domain of the discrete wavelet transform of the pixel intensity curves. We show improvements of our multiscale method, based on complexity-penalised likelihood estimation for Recursive Dyadic Partitioning of the image, over existing monoscale approaches, by simulated and real data examples, and we give some theoretical treatment of the resulting misclassification rate in the simplified set-up of the "horizon" model of two classes. This is joint work with J. Bigot (Toulouse) and A. Antoniadis (Grenoble).

Wavelet smoothing by ℓ_ν penalized likelihood for adaptive sparsity. **Sylvain Sardy** (École Polytechnique Fédérale de Lausanne, Switzerland) IC/MT403/010

For the problem of estimating possibly sparse sequences, we derive an information criterion based on the sparsity and asymptotic properties of likelihood estimators constrained in an ℓ_ν-ball, a natural measure of sparsity for $\nu \in [0,1]$. The ability of choosing ν adaptively allows for adaptive sparsity. Applying the ℓ_ν-ball model and estimation independently to each wavelet scale leads to a wavelet smoother that has comparable predictive performances to EBayesThresh.

Change-point oriented multiscale analysis using the lifting scheme. **Maarten Jansen** (Katholieke Universiteit Leuven, Belgium) IC/MT982/010

Recent developments in multiscale analysis include non-linear and adaptive data decompositions. One possible tool in the construction of data-adaptive multiresolution transforms is the lifting scheme. In the first instance, the lifting scheme decomposes the successive steps of a wavelet transform into smaller, immedidately invertible substeps. As the substeps are immediatly invertible, it is fairly easy to explore nonlinear and adaptive alternatives. We present a decomposition where the details at given scale not only carry information on feautures at that scale, but also directional information of where to look for features at forthcoming, finer scales. This is realized by adding a directional interpretation to the detail (say, wavelet) coefficients. Instead of simply adding a linear combination of a refinement basis (the wavelet basis) to the current approximation, the refinement now takes place in a direction perpendicular on the current approximating curve. It can be verified that this strategy localizes sharp transitions in the data. The resulting *normal offset* decomposition is highly non-linear and edge-adaptive. Due to this non-linearity, the decomposition must proceed from coarse scales to fine ones (whereas the wavelet transform itself proceeds the other way around). Moreover, it is important that the transform is numerically stable. Without numerical stability, the reconstruction from modified coefficients (e.g., thresholded coefficients in noise reduction) is not guaranteed to be close to the input data. The combination of numerical stability and the coarse-to-scale nature of the decomposition limits the degrees of freedom for the transform. We discuss what sort of wavelet transforms can be extended into non-linear normal offset transforms. We then illustrate the sharp edge reconstruction in an example of noise reduction.

IC/MP180/010: Multiscale models and methods for inference. #2

Organiser: Sofia Olhede (Imperial College London, UK)

(For abstract, see session #1 above.)

A wavelet/lifting scheme based imputation method. **Tim Heaton** (University of Oxford, UK), Bernard Silverman (University of Oxford, UK) IC/CT4415/010

It is often the case when performing a spatial survey that there exist sites of interest for which the underlying function is unobserved. In this talk we develop a new method to impute the value at these sites given information from neighbouring observed sites. Our approach takes advantage of the typically sparse representation of the underlying function in the wavelet domain within a Gibbs sampler framework. We illustrate our method on both regularly spaced one-dimensional data with the classical wavelet transform as well as irregularly spaced two-dimensional data using a Voronoi based lifting scheme. In particular we consider the estimation of rainfall in the US where we compare performance of our wavelet technique to the now standard approaches of thin plate splines and kriging.

Wavelet estimation of linear regression models. **Marina Vannucci** (Texas A&M University, USA) IC/MT2590/010

This talk will consider linear regression models where the error term is long memory. Data from long memory processes have the distinctive feature that the correlation between distant observations is not negligible. Wavelets, being self-similar, have a strong connection to long memory processes and have proven to be a powerful tool for the analysis and synthesis of data from such processes. Here, in particular, we will employ discrete wavelet transforms to simplify the dense variance-covariance matrix of the error structure. We will assume general Gaussian ARFIMA(p,d,q), autoregressive fractionally integrated moving average models, for the error term. We will allow unknown autoregressive and moving average parameters. Efficient recursive algorithms will help us to compute the variances of the wavelet coefficients. These will depend on the unknown characteristic parameters of the model. Markov chain Monte Carlo methods and direct numerical integration for inference will be designed. We will also consider alternative estimation techniques based on EM methods. Performances will be initially evaluated on simulated data. Linear regression models with long memory errors have proven useful for applications in many areas, such as medical imaging, signal processing, and econometrics. Recent successful applications include fMRI image data, and in this talk we will consider experimental data from human cognitive tasks.

The wavelet-Fisz transform. **Guy Nason** (University of Bristol, UK) IC/MT1793/010

The Haar-Fisz transform has been recently introduced as a technique for variance stabilization and 'Gaussianization' for various kinds of data. For example, for Poisson sequences one can effectively stabilize and normalize by taking the Haar wavelet transform and then dividing the wavelet coefficients by a function of the father wavelet coefficients (the Fisz transform) and then inverting. The idea can be extended to many situations such as spectrum estimation and also to where the distribution is not known but key information concerning the mean-variance function of the data can be estimated (the 'data-driven' Haar-Fisz transform). This talk will focus on a mathematical assessment of the wavelet-Fisz transform and to begin to explain why it works well for several interesting problems.

IC/MP444/010: Numerical solutions of Markov chains: techniques and applications.

Organiser: Evgenia Smirni (College of William and Mary, USA)
Co-organiser: Andreas Stathopoulos (College of William and Mary, USA)

Markov chains persist as the modeling tool of choice in a host of application areas ranging from performance evaluation of computer and communications systems to areas such as software verification and search engines. Despite tremendous advances in the techniques for solving Markov chains, the problems encountered in this area continue unabated. There are three reasons for this: The first is the state space explosion; adding small complexity to a system often increases exponentially the number of possible states to be described with a Markov chain. The second reason is that better numerical techniques and increasing computing power have allowed a more accurate modeling of various systems, for which lower quality approximations were acceptable until recently. The third reason is that the same computing power can be used to solve the simplified models on-line, making intelligent resource allocation decisions when these are needed.

To overcome these scalability and efficiency problems, researchers have developed ingenious algorithms and data structures, more efficient and robust numerical methods, and often new theories that attempt to avoid numerical solutions through appropriate statistical arguments. In this minisymposium, we bring together researchers that represent the state-of-the-art in both applications and methods areas. Three researchers will talk about data-structures and fitting techniques that attempt to curb the state explosion problem, and how this finds interesting applications in software verification. Statistical arguments will also be used to present closed form solutions in the context of QBDs. Efficient solution of continuous time Markov chains will be covered, as well as computing transient measures. A fluid queue approach will be presented, which is important in modeling network traffic. Talks about methods and their numerical properties will complement this minisymposium.

Shift techniques for the numerical solution of Markov chains. **Beatrice Meini** (Università di Pisa, Italy) IC/MT1402/010

Discrete-time Markov chains are characterized by stochastic matrices; i.e, non-negative matrices such that $Pe = e$, where e is the vector of all ones. The shift technique applied to a stochastic matrix P consists in performing a rank-one modification to P; i.e., $Q = P - ev^T$ where v is an arbitrary vector such that $v^T e = 1$. If P is irreducible and primitive, we may show that Q has spectral radius less than one, moreover its eigenvalues concide with the eigenvalues of P, except for the eigenvalue 1 which is shifted to 0. We show some applications of the shift technique in the numerical solution of structured Markov chains.

A first application arises in the analysis of $M/G/1$-type Markov chains. Here a fundamental problem is the computation of a stochastic matrix G, which solves a suitable nonlinear matrix equation. The shift technique is applied to G, and a nonlinear matrix equation is solved for a matrix $H = G - ev^T$ having spectral radius less than 1.

A second application is the solution of a nonsymmetric algebraic Riccati equation arising in fluid queues. The coefficients of the Riccati equation form a singular M-matrix M. The shift techique is applied to move one zero eigenvalue of M to a suitable nonzero real number.

In both applications, the convergence of existing algorithms is accelerated when the algorithms are applied to the shifted problems.

Assessing transient performance measures of infinite structured Markov chains using steady state techniques. **Benny Van Houdt** (Universiteit Antwerp, Belgium) IC/MT2183/010

This talk features a recent methodology to derive transient performance measures for a broad class infinite structured Markov chains. The main concept of this methodology exists in extending the Markov chain with a mechanism that marks some time epochs according to a set of Markovian rules.

Our interest lies in characterizing the system state at the n-th marked time epoch as well as the mean time at which this n-th marking occurs. The methodology transforms this transient problem into a stationary one by applying a (discrete) Erlangization and constructing a reset Markov chain.

In a second step, we specifically focus on the following classes of discrete and continuous time bivariate Markov chains (MC): Quasi-Birth-and-Death (QBD) MCs, M/G/1- and GI/M/1-type MCs, as well as MCs with a tree-structured state space, being tree-like processes. For each of these classes, a fast algorithm, with limited memory usage, that exploits the block structure of the reset Markov chain to a high degree is developed and is based, among others, on Sylvester matrix equations and fast Fourier transforms.

Attention is also paid to the computational effort required when studying the impact of several possible initial configurations. It is demonstrated that most of the computational work needed for one specific initial system state, can be reused during the computation for subsequent initial states.

Some numerical examples in the area of telecommunication systems are also provided.

Explicit solutions for a general class of Markov processes. **Mark Squillante** (IBM T.J. Watson Research Center, USA), Johan Leeuwaarden (EURANDOM, The Netherlands), Erik Winands (Technische Universiteit Eindhoven, The Netherlands) IC/MT3788/010

We consider a general class of infinite multidimensional Markov processes and derive explicit solutions for their stationary distribution and tail asymptotics. More specifically, we present an exact matrix-geometric solution for the stationary probability vector. We reformulate the probabilistic interpretations of the fundamental solution matrices in terms of Bernoulli excursions, leading to explicit expressions for these matrix elements in terms of hypergeometric functions. We establish asymptotic results on the powers of one of the fundamental solution matrices, which are used together with the corresponding matrix element expressions to obtain explicit large-deviation decay rates.

Bridging ETAQA and Ramaswami's formula for the solution of $M/G/1$-type processes. **Evgenia Smirni** (College of William and Mary, USA), Andreas Stathopoulos (College of William and Mary, USA) IC/MT3780/010

For some time, the method of Ramaswami has been the established way to analyze $M/G/1$-type processes. The ETAQA method, proposed previously, has offered a more efficient alternative for the exact computation of a general class of metrics for $M/G/1$-type processes. However, the stability of ETAQA and its relation to Ramaswami's method were not well understood.

Here, we derive a new formulation that improves the numerical stability and computational performance of ETAQA. As with ETAQA, the resulting methodology which we call newETAQA, solves a homogeneous system of equations to obtain the aggregate probability of a finite set of classes of states from the state space. In contrast to ETAQA, newETAQA constructs its matrix X in a way similar to the method of Ramaswami, decoupling the computation of the probabilities of the first two initial classes of states from the computation of the aggregate probability. Because direct methods are used to solve this system, the decoupling implies an often significant speedup over ETAQA. In addition, we show that the matrix X is an M-matrix, and under certain conditions, X is also diagonally dominant and thus can be factored stably. More importantly, we show that the newETAQA method is just an efficient way to implement Ramaswami's method. We also discuss alternative normalization conditions for Ramaswami's method.

Our numerical experiments demonstrate the stability of our method for both stiff and well behaved processes, and for both low and high system utilizations.

IC/MP444/010: Numerical solutions of Markov chains: techniques and applications. #2

Organiser: Evgenia Smirni (College of William and Mary, USA)
Co-organiser: Andreas Stathopoulos (College of William and Mary, USA)

(For abstract, see session #1 above.)

Decision diagrams for the exact solution of Markov models. **Andrew Miner** (Iowa State University, USA) IC/MT3412/010

High-level models of asynchronous systems can easily produce large Markov chains, whose solution is desired to determine performance measures about the system. Although these Markov chains are typically quite sparse, they can still require an excessive amount of storage space if a traditional, sparse matrix representation is used. This talk surveys compact data structures — namely decision diagrams, matrix diagrams, and Kronecker algebra — that can be used to generate and store extremely large Markov chains corresponding to a high-level description. Algorithms are presented for both generation and exact numerical analysis of a Markov chain, using these compact representations.

Decision diagrams for the approximate performance analysis of Markov models of distributed software. **Gianfranco Ciardo** (UC Riverside, USA) IC/MT3413/010

Decision diagrams of various types can be used to encode the exact state space and transition rate matrix of enormous Markov models. However, the exact solution of such models still requires to store at least one real vector with one entry per reachable state, a formidable limitation to the practical use of these encodings. Thus, we discuss automatic techniques for the approximate computation of performance measures when the Markov model can be compactly encoded but not exactly solved. We illustrate the proposed approximation techniques on an ideal target application, the computation of performance measures for a distributed software tasking system.

Markov fluid queue with application to the token bucket analysis. **Marie-Ange Remiche** (Université Libre de Bruxelles, Belgium) IC/MT2850/010

This talk outlines the recent advances for the analysis of the token bucket model for Markovian type traffic pattern. Our analysis makes extensively use of recent results about Markov driven fluid queue. Indeed, it has been shown these last years, that matrix-analytic methods were appropriate tools for the analysis of such a queue. Several efficient algorithms can actually be adapted for measuring the performance of such system.

We first define our token bucket model that is a Markov fluid queue with finite buffer and downwards jumps. Secondly, we clearly identify methods for its analysis and give some numerical results too.

Constructing compact Markov processes for correlated workload modeling. **Armin Heindl** (Universität Erlangen–Nürnberg, Germany) IC/MT2259/010

Unnecessarily large submodels aggravate the state-space explosion problem for Markov models. For example, large models often require various submodels for arrival and service processes, which, moreover, may exhibit correlations. Especially for computer and communication systems modeling, this is the case. The orders of these submodels may multiplicatively flow into the size of the overall model quickly leading to intractable state spaces. To mitigate this effect, compact and correlated Markov processes, in particular Markovian arrival processes (MAPs) of low order, have been developed, which can be used for workload modeling.

This talk discusses different ways how to construct MAPs from information on marginal moments and the autocorrelation function. A canonical form for MAPs of second-order is presented, by means of which we illustrate the flexibility of second-order matrix representations to capture correlation. Such canonical forms do not yet exist for higher dimensions. For this case, we give a brief overview of current approaches to obtain compact MAPs with given properties. Often, an inverse canonical form for matrix-exponential processes, which matches moments and correlation parameters, will play a key role.

IC/MP328/010: Clinical pathodynamics: dynamic modeling of disease in a stochastic system.

Organiser: Donald Trost (Pfizer Global Research and Development, USA)

Tremendous resources are being applied to health care and large amounts of data are collected on individuals undergoing medical observation and treatment. Yet little resource is being applied to the mathematical modeling of the whole human system. Most of clinical science and practice involves the gathering of data and the exercising of clinical judgment in the interpretation and application of these data, but there is little hard science. A more organized, mathematical framework for clinical science is needed.

Systems biology has become a popular topic. However, this is a bottom-up view and will take many years to consolidate into a coherent view of the organism. In the meantime, little progress will be made at the organism level, i.e., in the clinical setting, and medical practice will advance much more slowly than it would with the aid of mathematics.

While we wait for the orderly discovery and construction of the whole organism system, it seems that some significant contributions could be made by attacking the inverse problem, which is how clinical science has developed historically, although without much aid from mathematics. Using an astronomical analogy, clinically we are currently at the stage of Copernicus, Kepler, and Newton.

The primary idea behind pathodynamics is that the organism exists in a state of homeostasis, a dynamic equilibrium, and that dynamic changes from the homeostatic state occur naturally in diseases and artificially during therapeutic interventions or other external influences. One view is that the organism can be treated as a high-dimensional Brownian particle in a universe whose structure is unknown at present, where the dimensions are determined by clinically measurable quantities. Some of the underlying biological mechanisms may be inferred from observing and classifying the patterns of motion of this Brownian particle.

This session is intended to introduce some of these ideas and to stimulate research to advance clinical science.

An introduction to pathodynamics from the view of homeostasis and beyond. **Donald Trost** (Pfizer Global Research and Development, USA) IC/MT2940/010

The human body is a system of discrete and continuous signals. These signals are usually observed and measured by a physician or the physician's assistant or by some form of instrumentation. The diagnoses or clinical judgments are typically derived from changes of state: Change since the last observation, change from a statistical definition of normal, change from an intuitive sense of normal from training and experience, biological asymmetry, change reported by the patient, etc. Medical statisticians quantify these changes using counts, differences, time to an event, and sometimes empirical models relating several variables. These are typically averaged in some way and compared to a probability distribution for decision making. The variability is considered to be noise or a nuisance and is removed. The observed changes and the quantification methods tend to remove much of the biological information found in the variability of the signals. Somehow the dynamics of the system need to be quantified and used as the foundation for medical science.

The concept of Brownian motion was introduced by a biologist almost two centuries ago. Its mathematical foundations were developed by Einstein, Wiener, and others. Although it has been used extensively in statistical physics and mathematical finance, there are relatively few applications in biology and essentially none in clinical medicine. It seems like a natural place to start the study of biological system dynamics.

Homeostasis can be viewed as the state of dynamic equilibrium, while pathology, or more correctly a disease or iatrogenic state, can be viewed as a dynamic disequilibrium or a nonviable static state. This presentation discusses how dynamic models and Brownian motion methods can be applied to the analysis of clinical measurements. This approach has the potential to facilitate the understanding of biological systems on a macroscopic scale, much like thermodynamics did for physical chemistry.

Analysis of longitudinal clinical lab data with latent mixture models. **Jonathan Schildcrout** (Vanderbilt University, USA) IC/MT1474/010

In Phase I, II, and III clinical trials, laboratory data are collected routinely for the purpose of characterizing medication safety. However, for reporting, continuous data are often dichotomized at some threshold value (e.g., 3 times the upper limit of normal), and the longitudinal nature of the data (e.g., repeated measures on individuals) is ignored. Standard pre-marketing pharmaceutical safety analyses often compare the proportions of subjects who cross this threshold value 'at some point in time' during follow-up. Thus, much of the information collected is lost during analyses. Effective characterization of pharmaceutical safety requires analyses that can capture dynamic (and continuous) effects of treatments. By using longitudinal data analysis methods, we may capture mean response differences as functions of time; however in many situations, even those approaches are inadequate. For example, in a number of settings, a large proportion of subjects exhibit no response to treatment and fraction of subjects exhibit substantial responses. Thus, there appears to be some level of responsiveness that varies between subjects, and the information (e.g., genetic) that could explain such differences is unavailable. In such cases, standard longitudinal methods would likely produce a modest treatment effect estimate. In this talk, we will discuss models that posit underlying (latent) responsiveness indicator variables. By approaching analyses in this manner, we are able to address questions that neither the standard analytical methods for pharmaceutical safety nor longitudinal methods can address. Namely, we are able to estimate the probability of being a responder or a non-responder to treatment plus the longitudinal and dynamic treatment effect conditioned on being a responder. Several approaches will be considered, and all discussions will be focused on an analysis regarding the hepatotoxic effect of a single product.

Modeling laboratory measurements from clinical studies. **Gerd Rosenkranz** (Novartis Pharma AG, Switzerland) IC/MT3291/010

The analysis of laboratory measurements and other biomarkers in clinical studies is mainly done by means of data reduction: Often, the worst values from each individual patient are taken into consideration or the incidence of extremely high or low values observed during a trial. Where feasible, graphical representations of the time course of lab measurements are displayed, often for each subject individually. However, only rarely is the attempt made to model the dynamics of the measurements over time.

In this presentation we propose to model the dynamics of lab values by stochastic processes, preferably but not limited to (multivariate) Ornstein-Uhlenbeck processes. This should provide a means to account for potential systematic effects relevant for all or a group of subjects as well as the random variation between subjects. The idea is to estimate parameters of these processes from data in order to characterize a potential effect of drugs or other medical treatments compared to placebo. Results based on simulations and real data will be presented.

Statistical estimation of dynamic parameters in ODE models with applications to HIV and influenza virus infections. **Hulin Wu** (University of Rochester, USA) IC/MT3496/010

I will review the existing statistical methods and present several newly-developed methods for parameter estimation in ODE models based on the data from experiments and clinical studies of HIV and influenza virus. These dynamic parameters may include both constant parameters and time-varying parameters. The proposed estimation methods include the standard nonlinear least-squares method, a Bayesian method and more advanced statistical estimation methods that can avoid numerical evaluations of ODEs. The identifiability problems will be discussed. Real data examples will be presented to illustrate the methodologies and user-friendly software including both ODE simulations and statistical estimation modules will be introduced.

IC/MP3642/081: Advances on computation in financial mathematics.

Organiser: Abdul Khaliq (Middle Tennessee State University, USA)
Co-organiser: Qin Sheng (Baylor University, USA)

The aim of the mini-symposium is to highlight recent advances on computational methods in financial mathematics. Numerical PDE approach is discussed which provids a powerful tools and consistent frameworks for pricing and hedging complex derivatives. The mini-symposium will contain talks presenting new research in topics including, but not limited to, computatinal methods on stochastic volatility models, Jump diffusion models, and exotic options.

Highly-efficient numerical schemes for pricing exotic options. **Abdul Khaliq** (Middle Tennessee State University, USA) IC/MT705/081

Numerical schemes often develop inaccuracies when pricing financial derivatives with non-smooth payoffs, multiple strike prices, and discrete barrier options. Moreover, large errors may occur in estimating the hedging parameters. Averaging the initial data, shifting the grids, projection methods, and smoothing schemes have been tried to deal with the severe discontinuities in the computational domain when pricing and hedging such exotic options. These methods are not typically found sufficient to properly restore the expected behavior of the options. We present a strongly stable (L-stable) and highly accurate method for pricing exotic options. The method is based on Padé schemes and also utilizes partial fraction decomposition to address issues regarding accuracy and computational efficiency. Non-smooth payoffs, which cause discontinuities in the solution, the standard methods are prone to produce large and spurious oscillations in the solution that mislead estimating options accurately. The proposed method does not suffer these drawbacks. The method is seen to be robust and reliable when applied to exotic options such as Complex digital options, Butterfly spread and Barrier options in one and two assets.

Numerical valuation of performance-dependent options. **Thomas Gerstner** (Universität Bonn, Germany) IC/MT374/010

The efficient and accurate valuation of financial derivatives is a central topic in computational finance. Performance-dependent options are an important class of derivatives whose payoff depends on the performance of one asset in comparison to other assets. The fair price of such options can be determined by the martingale approach as a multidimensional integral whose dimension is the number of assets under consideration. Usually, the integrand is discontinuous, though, which makes accurate solutions difficult to achieve by numerical approaches.

For performance-dependent options, we derive a representation of the solution which only involves the evaluation of several multivariate normal distributions. This solution uses novel tools from computational geometry which faciliate the fast enumeration of all cells in a hyperplane arrangement and its orthant decomposition. We show that the arising normal distributions can be efficiently computed using sparse grid quadrature methods. This way, the complexity and the dimensionality of the integration problem can be significantly reduced which allows the efficient pricing of performance-dependent options even for large benchmarks, which is illustrated in several numerical examples.

This research is joint work with Markus Holtz, University of Bonn

Software issues in wavelet analysis of financial data. **Robert Tong** (NAG Ltd, UK) IC/MT1581/081

Wavelet Multiresolution Analysis (WMA) is a tool that is widely applied in many areas of data processing, including financial time series. By revealing the structure of the data at multiple scales, the results of WMA can be used to challenge or confirm underlying assumptions of market models. In many cases, the software used to compute these analyses will have been provided by a third party. We examine here the requirements this imposes on the design and implementation of such software, together with possible limitations which should be taken into account by the user. An important aspect is the desirability of consistent output between different implementations in order to enable valid comparisons to be made. Further, the needs of users to choose an appropriate wavelet basis and produce results relevant to their application must be translated into efficient software in terms of scalability and the pre- and post-processing of data sets. These issues are illustrated with reference to applications such as Foreign Exchange rates.

A semi-smooth Newton method for an inverse problem in option pricing. **Bertram Düring** (TU Wien, Austria), Stefan Volkwein (Universität Graz, Austria), Jüngel Ansgar (TU Wien, Austria) IC/MT1287/081

We present an optimal control approach using a Lagrangian framework to identify local volatility functions from given option prices. We employ a globalized sequential quadratic programming algorithm and implement a line search strategy. The linear-quadratic optimal control problems in each iteration are solved by a primal-dual active set strategy which leads to a semi-smooth Newton method. We present first- and second-order analysis as well as numerical results.

IC/MP3642/081: Advances on computation in financial mathematics. #2

Organiser: Abdul Khaliq (Middle Tennessee State University, USA)
Co-organiser: Qin Sheng (Baylor University, USA)

(For abstract, see session #1 above.)

A direct method for pricing American-style derivatives. **Sebastian Quecke** (Universität zu Köln, Germany) IC/MT977/081

We propose a direct approach for pricing options with early exercise features under fairly general models of the underlying (including Lévy processes). The model of the underlying is described by the conditional probability densities of returns. Risk neutral valuation leads to a nested integral representation of the option price. Using radial basis functions we can compute this price efficiently. The method can also be applied to higher dimensional pricing problems. We present several numerical examples to illustrate the range of applications.

Computation of risk contribution in the Vasicek portfolio credit loss model. **Xinzheng Huang** (TU Delft, The Netherlands) IC/MT1206/081

A risk contribution in the context of portfolio credit loss modeling measures how much each obligor in a portfolio contributes to the total risk. The determination of risk contribution is of practical importance because it is necessary for loan pricing and it can provide limits on large credit exposures. It may also be useful for profitability assessment, asset allocation and portfolio optimization. Within the framework of the Vasicek portfolio credit loss model, we review several methods for the calculation of the marginal risk contribution, among others are importance sampling and saddlepoint approximations. Comparison of different methods are further illustrated by numerical examples.

This is joint work with Cornelis W. Oosterlee and J.A.M. van der Weide.

On the smoothing of Crank–Nicolson method and higher-order methods for pricing barrier-options. **Muhammad Yousuf** (King Fahd University, Saudi Arabia) IC/MT1507/081

Most option pricing problems have nonsmooth payoffs or discontinuous derivatives at the exercise price. Discrete barrier options have not only nonsmooth payoffs but also time dependent discontinuities. In pricing barrier options, certain aspects such as un wanted oscillations are triggered if the asset price becomes too high or too low. Standard smoothing schemes used to solve problems with nonsmooth payoff do not work well for discrete barrier options because of discontinuities introduced in the time domain when each barrier is applied. Moreover, these unwanted oscillations become worse when estimating the hedging parameters, e.g., Delta and Gamma. We have an improved smoothing strategy for the Crank-Nicolson method which is unique in achieving optimal order convergence for barrier option problems. Numerical experiments are discussed for one asset and two asset problems. Time evolution graphs are obtained for one asset problems to show how option prices change with respect to time. The smoothing strategy is then extended to higher order methods using diagonal (m, m) Padé as main schemes, and under a smoothing strategy of using as damping schemes the (0, 2m-1) subdiagonal Padé schemes.

Multi-asset option pricing using radial basis functions . **Sônia Gomes** (Universidade Estadual de Campinas, Brazil), Ulrika Pettersson (Uppsala University, Sweden), Elisabeth Larsson (Uppsala University, Sweden) IC/MT1190/081

The price for a multi-asset option can be computed through solution of a high-dimensional PDE problem, where the number of dimensions correspond to the number of underlying assets. Radial basis function (RBF) methods are attractive in this context because they are meshfree and because they can be spectrally accurate, thus reducing the number of unknowns needed. However, we have found that the performance of the RBF method for a typical problem, such as a European basket call option, is sensitive with respect to the placement of center and collocation points. Furthermore, an unnecessarily high resolution is needed due to the discontinuous derivative in the contract function. In this talk we show what benefits can be gained from using least squares approximation instead of collocation with RBFs.

IC/MP219/010: Advances on modeling in financial mathematics.

Organiser: Abdul Khaliq (Middle Tennessee State University, USA)
Co-organiser: Qin Sheng (Baylor University, USA)

The aim of the mini-symposium is to highlight recent advances on mathematical modeling in financial mathematics. PDE and Monte Carlo approaches are discussed which provide powerful tools and consistent frameworks for pricing and hedging complex derivatives. The mini-symposium will contain talks presenting new research in topics including, but not limited to, stochastic volatility models, regime switching, credit risks, and multi scale models.

Homogeneous groups and multiscale intensity models for multiname credit derivatives. **Ronnie Sircar** (Princeton University, USA) IC/MT1340/081

The pricing of basket credit derivatives is contingent upon (i) a realistic modeling of the firms' default times and the correlation between them; and (ii) efficient computational methods for computing the portfolio loss distribution from the firms' marginal default time distributions. We revisit intensity-based models, and with the aforementioned issues in mind we propose improvements ii) via incorporating fast mean-reverting stochastic volatility on the default intensity processes; and iiii) by considering a hybrid of a top-down and a bottom-up model with homogeneous groups within the original set of firms. We present a calibration example, and discuss the relative performance of the approach.

This is joint work with Evan Papageorgiou.

Multi-level quasi-Monte-Carlo path calculations for finance. **Michael Giles** (University of Oxford, UK), Ben Waterhouse (University of New South Wales, Australia) IC/MT1134/081

In this talk we will present advances in the multilevel Monte Carlo approach recently introduced for estimating expectations arising from stochastic path simulations. One focus is on improvements in both complexity and actual computational cost using Milstein's method instead of the Euler-Maruyama discretisation. In this context, particular attention is paid to the treatment of lookback, barrier and digital options. The second focus is on the introduction of Quasi-Monte Carlo techniques, in particular lattice rules and Sobol sequences. This leads to further substantial computational savings, yielding a very practical method for a wide range of option pricing applications.

Calibration of forward rate volatility in a Bayesian framework. **Christoph Reisinger** (University of Oxford, UK) IC/MT1141/081

The objective of this talk is the calibration of a time-homogeneous, hump-shaped volatility function to a time series of LIBOR rates. The observed data are used to estimate simultaneously the distribution of forward rates as unobservable driving processes, and the model parameters. Acknowledging the presence of observation noise in a Bayesian setting, we obtain parameter distributions that yield stable and accurate estimates together with measures for their uncertainty. This is joint work with Hugo Para, extending recent work by Bhar, Chiarella, Hung and Runggaldier.

Finite-horizon portfolio selection with transaction costs. **Min Dai** (National University of Singapore) IC/MT511/010

This paper concerns portfolio selection of a CRRA investor who faces proportional transaction costs and finite time horizon. From the angle of stochastic control, it is a singular control problem, whose value function is governed by a time-dependent HJB equation with gradient constraints. We reveal that the problem is equivalent to a parabolic double obstacle problem involving two free boundaries that correspond to the optimal buying and selling policies. This enables us to make use of the well developed theory of obstacle problem to attack the problem. The $C^{2,1}$ regularity of the value function is proven and the optimal investment policies are completely characterized. Relying on the double obstacle problem, we extend the binomial method widely used in option pricing to determine the optimal investment policies. Numerical examples are presented as well.

IC/MP219/010: Advances on modeling in financial mathematics. #2

Organiser: Abdul Khaliq (Middle Tennessee State University, USA)
Co-organiser: Qin Sheng (Baylor University, USA)

(For abstract, see session #1 above.)

Multiname and multiscale default modeling. **Knut Solna** (University of California, Irvine, USA) IC/MT1638/081

We consider multiname default modeling using a reduced-form modeling approach. The model is based on a multiscale model for the hazard rates of the underlying names. Such default modeling is important in the context of pricing for instance Collaterized Debt Obligations (CDOs) and we analyze the impact of volatility time scales on the default distribution and CDO prices.

The Heston stochastic-volatility model: parameter estimation through maximum likelihood and filtering. **Francesco Zirilli** (Università degli Studi di Roma "La Sapienza", Italy) IC/MT956/081

Let us suppose that the dynamics of the stock prices and of their stochastic variance is described by the Heston model, that is by a system of two stochastic differential equations with a suitable initial condition. The aim of this paper is to estimate the parameters of the Heston model and one component of the initial condition, that is the initial stochastic variance, from the knowledge of the stock and option prices observed at discrete times. The option prices considered refer to an European call on the stock whose prices are described by the Heston model. The method proposed to solve this problem is based on a filtering technique to construct a likelihood function and on the maximization of the likelihood function obtained. The estimated parameters and initial value component are characterized as being a maximizer of the likelihood function subject to some constraints.

The solution of the filtering problem, used to construct the likelihood function, is based on an integral representation of the fundamental solution of the Fokker–Planck equation associated to the Heston model, on the use of a wavelet expansion to approximate the integral kernel appearing in the representation formula of the fundamental solution, on a simple truncation procedure to exploit the sparsifying properties of the wavelet expansion and on the use of the Fast Fourier Transform (FFT). The use of these techniques generates a very efficient and fully parallelizable numerical procedure to solve the filtering problem, this last fact makes possible to evaluate very efficiently the likelihood function and its gradient. As a byproduct of the solution of the filtering problem we have developed a stochastic variance tracking technique that gives very good results in numerical experiments.

The maximum likelihood problem used in the estimation procedure is a low dimensional constrained optimization problem, its solution with ad hoc techniques is justified by the computational cost of evaluating the likelihood function and its gradient. We use parallel computing and a variable metric steepest ascent method to solve the maximum likelihood problem. Some numerical examples of the estimation problem using synthetic and real data, that is data relative to an index of the Milano stock exchange (S&PMIB3O), obtained with a parallel implementation of the previous numerical method are presented. Very impressive speed up factors are obtained in the numerical examples using the parallel implementation of the numerical method proposed. The website: http://www.econ.univpm.it/pacelli/mariani/finance/w1 contains animations and some auxiliary material that helps the understanding of this paper and makes available to the interested users the computer programs used to produce the numerical experience presented.

An optimal variance reduction method for density estimation. **Ahmed Kebaier** (Université de Paris–Dauphine, France), Arturo Kohatsu-Higa (, Japan) IC/MT1549/081

This work is in collaboration with Arturo Kohatsu-Higa. We study the problem of density estimation for non-degenerate diffusions using kernel functions. Thanks to Malliavin calculus technics, we obtain an expansion of the discretisation error. Then, we introduce a new control variate method in order to reduce the variance in the density estimation. We prove a stable law convergence theorem of type Jacod Kurtz Protter, for the Malliavin derivative of the error process, which leads us to get a CLT for the new variance reduction algorithm. This CLT gives us a precise description of the optimal parameters of the method. The numerical results confirm the efficiency of the method.

American options in regime switching Levy models. **Sergei Levendorskiĭ** (University of Texas at Austin, USA), Svetlana Boyarchenko (University of Texas at Austin, USA) IC/MT499/010

In the talk, a general framework for pricing of perpetual American and real options in regime-switching Lévy models is presented. In each state of the Markov chain, which determines switches from one Lévy process to another, the payoff stream is a monotone function of the Lévy process labelled by the state. This allows for additional switching within each state of the Markov chain (payoffs can be different in different regions of the real line). The payoffs and riskless rates may depend on a state, which allows for jumps in prices at moment of switching. Special cases are stochastic volatility models and models with stochastic interest rate; both must be modelled as finite-state Markov chains. We construct iteration procedures and prove that iterations converge to the solution of the optimization problem monotonically. The procedures are numerically efficient even if the number of states is large provided the transition rates are not large w.r.t. the riskless rates. As first applications, we solve exit problems for a price-taking firm, and pricing problems for American options with infinite and finite time horizon. In the latter case, we use a modification of Carr's randomization procedure for regime-switching models.

IC/MP1894/081: Financial modeling with jump processes.

Organiser: Christoph Schwab (ETH Zürich, Switzerland)
Co-organiser: Rama Cont (Columbia University, USA)

In the past decade, financial models with jump processes have become widely accepted as generalization of the classical Black–Scholes models.

This minisymposium will review some of the latest developments in this area, in particular:

- multidimensional models with jumps: dependence modeling, Lévy copulas, numerical methods for multidimensional models;
- simulation and estimation: efficient simulation of multivariate models, econometrics of jump processes, realized volatility/bi-power variation;
- partial integro-differential equations (PIDEs) and computational methods;
- interest rate and credit risk models with jumps and their efficient analytical and numerical treatment.

Recovering Levy processes from option prices: stable algorithms for an ill-posed inverse problem. **Rama Cont** (Columbia University, USA) IC/MT2921/081

In the class of exponential Lévy models, where the risk neutral dynamics of an asset price S_t is expressed as $S_t = \exp X_t$ where X_t is a Lévy process determined by its Lévy triplet (b, σ, ν) where $\sigma \geq 0$, ν is a Radon measure on $\mathbb{R} - \{0\}$ with $\int \nu(dx)(1 \wedge x^2) < \infty$. Option prices in this model can be characterized as solutions of partial integro-differential equations (PIDEs). A preliminary step in using the model is to solve the following *inverse problem*:

Given a set of prices of call options $C(t, S, T_i, K_i), i \in I$, find $\sigma \geq 0$ and a Lévy measure ν such that

$$\forall i \in I, C(t, S, T_i, K_i) = e^{-r(T-t)} E^{(\sigma,\nu)}[(S(T_i) - K_i)^+ | S_t = S].$$

This is equivalent to an inverse problem for the corresponding partial integro-differential equation (PIDE). The issue is to find stable algorithms for solving this ill-posed inverse problem in the realistic case where the number of observations is finite.

After pointing out the drawbacks of standard parametric output least squares methods, we present various *nonparametric* approaches to this problem. The first, jointly developed with P. Tankov, is a regularization method based on relative entropy. The second, jointly developed with M. Rouis, uses Tikhonov regularization and computation of the solution by solving an adjoint PIDE. In each case we provide a theoretical analysis of the calibration algorithm, discuss numerical implementation issues and assess their empirical performance using market data.

Finally, we discuss issues related to calibration of American options, which lead to inverse problems for free-boundary PIDEs.

Time-changed intensity models for portfolio credit risk. **Philipp Schönbucher** (ETH Zürich, Switzerland) IC/MT2022/081

In this paper, we present a general methodology to introduce dependence in multivariate intensity-based credit risk models using stochastic time changes of the underlying processes. We analyze the properties of the resulting models, compare them to existing multivariate intensity-based credit risk models and present an efficient methodology for the numerical implementation and calibration of such models.

Hedging options in presence of jumps. **Peter Tankov** (Université Paris VII, France), Rama Cont (Columbia University, USA), Ekaterina Voltchkova (Université Toulouse I, France) IC/MT2207/081

We study the problem of hedging options when the underlying asset is described by a process with jumps. We compare various hedging strategies using the underlying asset and a set of liquid options and examine the properties of the hedging error, both theoretically and through numerical experiments. We illustrate in particular that using *sensitivities* to compute Δ-neutral and Γ-neutral hedge ratios can lead to a large hedging error, and illustrate how such strategies can be improved by using a risk-minimizing approach to hedging and by taking positions in options.

Keywords: option pricing, hedging, integro-differential equations, finite difference methods, Lévy process, jump-diffusion models.

Pricing of financial derivatives using multivariate jump processes. **Christoph Winter** (ETH Zürich, Switzerland) IC/MT4579/081

For one-dimensional Lévy processes option pricing by solving the corresponding partial integro-differential equations has been studied by several authors. We extend the results to multivariate jump processes using Lévy copulas. The partial integrodifferential equations are discretized by sparse tensor product Finite Element spaces. Since the multi-dimensional tail integrals have singularities at the origin and on the axes, variable order composite quadrature formulas are employed for the computation of the integral part. Numerical examples are given.

This is joint work with N. Reich.

IC/MP306/013: Recent developments in the stochastic exit problem.

Organiser: Samuel Herrmann (École des Mines Nancy, France)
Co-organiser: Nils Berglund (Centre de Physique Théorique - CNRS, France)

The escape of a Brownian particle from a potential well, under the influence of external noise, was studied by Eyring and Kramers in the 1930s. The mathematical formulation of the phenomenon leads to the so-called stochastic exit problem. Consider a diffusion process, described by the Itô stochastic differential equation

$$\mathrm{d}X_t^\epsilon = b(X_t^\epsilon)\mathrm{d}t + \sqrt{\epsilon}\sigma(X_t^\epsilon)\mathrm{d}W_t\,,$$

where the noise intensity ϵ is a small parameter, and W_t is a Brownian motion in $\mathbb{R}^d$. Given a bounded domain $D \subset \mathbb{R}^d$, the exit problem consists in determining the small-ϵ asymptotics of the distribution of the first-exit time

$$\tau^\epsilon = \inf\{t > 0 :\ X_t^\epsilon \notin D\},$$

and of the exit location X_{τ^ϵ}.

Since the first rigorous results were obtained by Freidlin and Wentzell in the late 1960s, using techniques from the theory of large deviations, the problem has been addressed by a variety of rigorous approaches, including formal and systematic asymptotic expansions and potential theory, as well as by various numerical techniques.

The results are relevant for many applications: modern communication systems, stochastic stability of structures, modern theory of finance, climate models, the dynamics of macromolecules, metastability, stochastic resonance, etc.

The aim of this minisymposium is to present recent developments in the classical exit problem, including precise subexponential asymptotics for gradient systems, cycling and skewing phenomena for nongradient systems, and their applications, but also recent results for more general types of noise.

Small eigenvalues of reversible diffusions in the metastable regime. **Michael Eckhoff** (Universität Erlangen–Nürnberg, Germany) IC/MT3995/0

For generic $F : \mathbb{R}^d \to \mathbb{R}$ with finitely-many local minima and Brownian motion $(W_t, t \geq 0)$ the randomly perturbed dynamical system

$$dX_t = -\nabla F(X_t)dt + (2\varepsilon)^{1/2}dW_t, \quad \varepsilon > 0,$$

exhibits several quasi-invariant states corresponding to the local minima on the long term run as ε becomes small. They determine the in $1/\varepsilon$ exponentially small eigenvalues of the generator and are given in a precise way as the inverse of expected relaxation times of the corresponding quasi-invariant states. Their rescaled distribution functions converge uniformly to that of an exponential random variable.

Large fluctuations, classical activation, quantum tunneling, and phase transitions. **Daniel Stein** (New York University, USA) IC/MT3677/0

I will discuss two broad classes of physically dissimilar problems, each corresponding to stochastically driven escape from a potential well. The first class, often used to model noise-induced order parameter reversal, comprises Ginzburg-Landau-type field theories defined on finite intervals, perturbed by thermal or other classical spatiotemporal noise. I will present recent results from collaborative efforts applying our theory of escape in these types of systems to two different problems: the thermally induced breakup of monovalent metallic nanowires, and stochastic reversal of magnetization in thin ferromagnetic annuli.

The second class comprises systems in which a single degree of freedom is perturbed by both thermal and quantum noise. Each of the two above classes of problem possesses a transition in its escape behavior, at a critical value of interval length and temperature, respectively. It is shown that there exists a mapping from one class of problems to the other, and that their respective transitions can be understood within a unified theoretical context. Finally, I will explore the depth of the analogy between the two classes of problems, and discuss to what extent each case exhibits the characteristic signs of critical behavior at a sharp second-order phase transition.

Dynamical systems with heavy-tail Levy noise. **Ilya Pavlyukevich** (Humboldt University Berlin, Germany) IC/MT3679/0

We consider a dynamical system in $\mathbb{R}$ driven by a vector field $-U'$, where U is a multi-well potential satisfying some regularity conditions. This dynamical system is perturbed by a heavy-tail Lévy noise of small intensity. For the perturbed system, we determine the law and mean value of the transition times between potential wells and formulate results on metastablity. We also discuss how global optimisation problems can be solved with help of simulated annealing with big jumps.

Simulation of exit times and positions for the Brownian motion and diffusions. **Madalina Deaconu** (INRIA Lorraine, France), Antoine Lejay (INRIA Lorraine, France) IC/MT3670/0

Monte Carlo methods are sometimes the only way to deal with some deterministic problems (solving some PDE, computing some effective coefficients). We present here some recent developement in the simulation of the Brownian motion and SDEs, that can be useful when one needs some precise estimation of the first exit times and positions from some domain, or when one whishes to estimates an exit probability which is small or the tail of the distribution function of the exit time. Applications will also be presented.

From joint works with Antoine Lejay (Projet OMEGA, Institut Elie Cartan, Nancy, France)

IC/MP299/010: Shape and size in medicine, biotechnology and material Science.

Organiser: Vincenzo Capasso (Università degli Studi di Milano, Italy)
Co-organiser: Alessandra Micheletti (Università degli Studi di Milano, Italy)

Shape analysis deals with the geometrical information on objects that is left after location, scale and rotation effects are removed. If scale effects are not removed, then we are led to form (size and shape). In applications, bodies rarely have exactly the same shape within measurement error; hence randomness of shapes need to be taken into account. Thanks to the development of information technologies, the last decade has seen a considerable growth of interest in the statistical theory of shape and its application to many and diverse scientific areas.

Often the diagnosis of a pathology, or the description of a biological process mainly depend on the shapes present in images of cells, organs, biological systems, etc., and mathematical models which relate the main features of these shapes with the correct outcome of the diagnosis, or with the main kinetic parameters of a biological systems are still not present. In material sciences optimisation for quality control require methods of statistical shape analysis.

From the mathematical point of view, shape analysis uses a variety of mathematical tools from differential geometry, geometric measure theory, stochastic geometry, etc. As far as applications are concerned, we emphasize here topics which are relevant in medicine, biotechnology and material sciences. We deal with direct and inverse problems. Among direct problems, spatio-temporal pattern formation deals with the analysis of how patterns are created and developed in biology. Among

inverse problems, various statistical techniques of shape analysis will be proposed to measure in a quantitative way the random variability of objects.

Variational surface matching and applications in medicine. **Hans Lamecker** (Zuse-Institut Berlin, Germany), Hans-Christian Hege (Zuse-Institut Berlin, Germany), Peter Deuflhard (Zuse-Institut Berlin, Germany) IC/MT1937/083

Shape matching or registration is a prerequisite for quantitative shape analysis. It is a fundamental ingredient for reconstruction, recovery, tracking, detection and transformation of shapes. These techniques are applied in fields such as computer graphics, computer vision, pattern recognition, robotics, image processing and many more, of which it is almost impossible to give full account.

In this talk, shape will be understood as geometric information of a three-dimensional object, i.e. we are only interested in the boundary representation of a given object, thereby neglecting its inner structure. The talk will focus on the task of comparing shapes. This task relies on the ability of identifying corresponding points on different shapes, which is often referred to as the *correspondence problem*. We will consider only inter-object registration. For this case, the usual elastic deformation approach based on "material properties" is not well-suited.

Two main challenges in establishing this correspondence between 3D shapes have to be faced: (1) to define a distance measure for characterization of the similarity of two surfaces and (2) to formulate, discretize and solve the correspondence problem directly.

(1) As for the distance measure, we will propose a functional for establishing correspondence between 3D shapes. It has been derived by invariance considerations and a purely differential-geometric characterization of shape, reflecting the fundamental theorem of surface theory.

(2) As for solving the correspondence problem, we show first steps toward an adaptive multilevel FE method associated with minimizing the proposed distance functional.

Among the large variety of potential applications of shape matching the talk will restrict its attention to statistical shape modeling. There, the idea is to capture the *essential degrees of freedom* of variations within a well-defined training database. Correct correspondence between shapes is essential in order to capture the true variability. Two important applications of statistical shape modeling in medicine will be presented:

(A) Atlas-based segmentation of 3D image data for oncological liver surgery. The segmentation of the liver tissue is an important prerequisite for liver surgery planning. In clinical routine, manual segmentation of the liver parenchyma is too time consuming (about one hour per data set). The segmentation time will be even longer with increasing number of slices from improved CT scanners. Therefore methods have to be devised that require little interaction time. We have developed a statistical 3D shape model of the liver tissue for the automatic segmentation of contrast enhanced CT data. The algorithm has been validated on more than 30 patient data sets acquired from different scanners, yielding an accuracy of about 2 mm average surface distance.

(B) Reconstruction of malformed shapes in cranial neurosurgery. Skull deformities can lead to increased intra-cranial pressure, vision, hearing, and breathing problems. Research on the correction of underlying disorders on the cellular level is still being carried out. Thus, patients with craniosynostosis currently depend on surgical intervention for preventing or reducing functional impairment and improving their appearance. A definition of the correct target shape after surgery is missing. The most important and in many cases only indication of the best possible approximation of the skull shape to the unknown healthy shape is left to the subjective aesthetic assessment of the surgeon. This prevents impartial control of therapeutic success and aggravates guidance and instruction of the remodeling process for inexperienced surgeons. A statistical shape model of the cranium was created from 21 MRI data sets. In a first clinical application, the statistical model was pre-operatively matched to a patient and taken to the operating room to assist the reshaping process.

New level-set techniques for the crack-detection problem. **Diego Álvarez** (Universidad Carlos III de Madrid, Spain), Oliver Dorn (Universidad Carlos III de Madrid, Spain), Miguel Moscoso (Universidad Carlos III de Madrid, Spain) IC/MT4114/083

In this talk we address the problem of detecting thin cracks from boundary data. The cracks are modeled as thin shapes of fixed thickness which need to be reconstructed from boundary electrical measurements. We introduce an extension of the level set technique for modelling these thin shapes. Two level set functions are employed for modelling these crack-type structures. The first one models the location and form of the crack, and the second one models its length and connectivity. A gradient based method is derived in order to define iterative updates for both level set functions with the goal to reduce and eventually minimize a given least squares data misfit functional. These successive corrections of the two level set functions correspond to an evolution of the thin shape or crack during the reconstruction. We present numerical experiments which demonstrate that our technique is able to recover disconnected thin shapes or cracks from noisy simulated boundary data.

The stochastic geometry of kinetic-driven crystallization processes: modelling, simulation and statistical analysis. **Stefano Patti** (Università degli Studi di Milano, Italy), Alessandra Micheletti (Università degli Studi di Milano, Italy), Vincenzo Capasso (Università degli Studi di Milano, Italy), Martin Burger (Universität Münster, Germany), Marco Rubbo (Dip.Scienze Mineralogiche e Petrologiche. Torino, Italy), Dino Aquilano (Università degli Studi di Torino, Italy) IC/MT4144/083

Crystal growth is a topic that has been widely studied by mathematicians and physicists. We propose a new model by taking account of kinetic contributions only; this model is coherent with the classical Stefan Problem proposed in the literature. In particular we solve numerically the case of multiple growth, by considering a stochastic contribution due to the random nucleations in time and in space; therefore a birth-and-growth process arises. The coupling of the growth dynamics with the evolution of the underlying field of the concentration of matter causes the stochastic geometry of the crystals, which present a strong spatial non homogeneity. Then we perform on the numerical simulations some measurements on the evolving geometry of the process, e.g. the size of the crystals, the volume fraction of the crystal phases, etc. Since some of these random quantities may be represented by random functions, we apply some functional data analysis techniques to solve the related statistical problems. In particular we perform a functional regression of the expected size of the crystals with respect to the kinetic parameters of growth.

Configurations of steps during growth limited by surface processes. **Marco Rubbo** (Dip.Scienze Mineralogiche e Petrologiche. Torino, Italy) IC/MT4171/083

The talk deals with the configuration of growth steps originated at the outcrop of a screw dislocation on a crystal face. These steps wind around the dislocation lines forming growth hillocks on a crystal face.To describe a growth hillock let's consider its intersection with a plane perpendicular to the crystal face: such intersection is a line consisting, in the crystal growth jargon, of terraces and rises (the steps). When seen on an orthogonal projection over the crystal face, the steps form a peculiar pattern, the so called growth spiral; the spiral arms are the steps projection and the distance between consecutive arms gives the width of the terraces. The profile of a hillock is defined by the set of terraces lengths and steps heights. The smallest height of a step is a property typical of each crystal face. From a physical point of view, the distance between steps depends on: -the kinetics of exchange of matter between the crystal and the mother phase, -the frequency of production of steps at the dislocation, -the kinetic interaction among growth hillocks; -other causes which are not affecting the main features of the model we are going to present. By kinetic interaction among growth hillocks we mean the overlap of the concentration fields of growth units around contiguous hillocks. That interaction determines the rate of the outer steps of the hillocks and this fact constrains the outer steps distance. When the distance between two consecutive steps becomes nil they coalesce in one step of multiple height. In order to model the transient configuration of the steps and to look for the existence of a steady state, we formulate a system of reaction-diffusion equations solved by a numerical method. We will present an up to date review of the different configurations of steps obtained, depending on the initial and boundary conditions chosen; moreover we will discuss their long term behaviour.

IC/MP299/010: Shape and size in medicine, biotechnology and material Science. #2

Organiser: Vincenzo Capasso (Università degli Studi di Milano, Italy)
Co-organiser: Alessandra Micheletti (Università degli Studi di Milano, Italy)

(For abstract, see session #1 above.)

The theory of size functions applied to problems of statistical shape analysis in bio-medicine. **Alessandra Micheletti** (Università degli Studi di Milano, Italy) IC/MT980/083

The solution to the problem of describing a *shape* via functions taking values in a finite-dimensional space, without loosing relevant information, is needed for the mathematical and statistical analysis of random objects. Recently new geometrical descriptors of shapes, the size functions, have been proposed. These functions are able to capture *globally* the geometric characteristics of an object, differently from landmarks (which usually are specific geometric descriptors, chosen by an expert), which are widely used in literature, but whose results in the statistical analysis are strongly dependent on their choice, leading to a sort of subjective quantitative analysis. Size functions depend on the choice of a measuring function, and usually only a small number of choices lead to different statistical results. The theory of size functions has been developed mainly in a deterministic framework. A first attempt of joining this theory with randomness and to develop the related statistical analysis is here presented. The approximation of size functions with their discrete counterpart leads to the formulation of suitable algorithms which may compute a graphical representation of the size function associated with a shape. The main features of the shape are thus described by a finite number of points and lines on a plane. The descriptor is robust, since small variations in the shape produce small variations in the location of such points and lines. Then confidence regions for different families of shapes, and thus solutions to classification problems can be provided via these tools. Applications to problems arising in biomedicine, in particular to the automatic classification of different types of tumor cells from their shape, will be presented.

Patterns and waves in some models of population dynamics with non-local consumption of resources. **Vitaly Volpert** (Université Claude Bernard Lyon I, France) IC/MT1791/083

We consider nonlinear integro-differential equations and systems of equations describing some problems in population dynamics with nonlocal consumption of resources. Their solutions show complex nonlinear dynamics with various patterns and waves. We study them in 1D and 2D cases. In the context of population dynamics the mechanism of pattern formation discussed in the present work can be related to intra-specific competition. The model provides a possible explanation of the emergence and of the evolution of biological species.

A brief overview of stereology: the art of geometric sampling. **Luis Cruz-Orive** (Universidad de Cantabria, Spain) IC/MT5007/083

Stereology is a interdisciplinary science which dictates rules of geometric sampling to estimate quantities defined on spatial objects (e.g. biological, or mineral structures) such as volume, number of cells, voids or inclusions, surface area, length of curvilinear structures, etc. The relevant information is the intersection between the object and a test probe of points, curves, planes, or full dimensional subsets with known geometric properties. The discipline providing the necessary link is integral geometry. The methodology borrows heavily from sampling theory, as opposed to reconstruction, and it applies to objects with no, or rather weak, assumptions about shape. Image analysis may play a role in data acquisition, but not in the sampling design. In design based stereology the object of interest is assumed to be non random, and unbiased estimation is warranted by a proper random mechanism for the probe hitting the object. This is the stereology applied to bounded objects, specially in biosciences. When probe replication is easily available unbiasedness is more important than precision, because the latter can be increased at will by increasing the sampling intensity. On the other hand, in model based stereology the object is regarded as a realization of a random closed set, usually stationary; in this case, the location of the probe may be arbitrary. Point process theory is a subsidiary discipline here. In all cases, the prediction of the variance due to sampling with systematic geometric probes, is usually a nontrivial, challenging problem. In the lecture an informal excursion is made to various aspects of stereology, with real examples.

Texture classification by statistical learning from morphological image processing. **Dominique Jeulin** (Ecole des Mines de Paris, France) IC/MT2387/083

The automatic extraction of objects in images is usually made by means of shape descriptors based on combinations of geometrical measurements (area, perimeter, size, orientation...) on already extracted objects. The optimal choice of parameters for shape classification can be obtained by multivariate statistical analysis of data obtained on populations of objects.

Complex images can contain various textures and defects, which cannot be easily extracted by a standard segmentation process, involving to develop very tedious algorithms valid for a single case of application.

In the present study, we propose a generic approach for the classification of textures, based on the use of morphological descriptors at the level of pixels. The mains steps of the approach are as follows.

- Each pixel of an image is described by a vector accounting for information in its neighborhood at different scales. Two families of descriptors are used at this level: the curvelets[2] and morphological sizings by opening and closing transformations [1]. Typically, the curvelets are obtained by a linear filtering of each 100×100 neighborhood of every pixel by 26 wavelets with different orientations and ranges. The morphological operators are non linear filters. The opening, obtained by an erosion followed by a dilation by a given structuring element, keeps bright parts of the image which can contain the structuring element, while the closing operation (dilation followed by an erosion) removed dark zones in an image. Increasing sizes of structuring elements are used, to cover the range $[2, 4, 8, 16, 32] \times 2 + 1$ in the present case. For a given type of structuring element (square, horizontal or vertical segment), we keep the difference between the open images at steps n and $n+1$, as well as between the closed images at steps $n+1$ and n. Therefore each pixel is described by a vector with 30 morphological components (5 sizes for 3 structuring elements and 2 operations), generating a file of 30 images.
- In a second step, every pixel is considered as an observation in a multidimensional space. Various techniques of multivariate statistical data analysis are used to generate a classification of pixels according to their environment: the PCA (principal components analysis), and the Kmeans algorithm (with a prior given number of classes)[3]. To avoid an over representation of pixels corresponding to dominant classes, a sampling of the pixels is generated for the multivariate analysis, and a classification of the pixels is performed according to their distance to the centers of the classes.
- In some cases, isolated pixels in the image can be affected to separate textures, generating noise in the segmentation. This is corrected by morphological filtering of the resulting image.

The approach is illustrated for two examples of applications in two different areas: the automatic extraction of textures and of defects on steel surfaces, and the texture based classification of biological cells.

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IC/MP77/008: Cointegrating, Kalman-filtering of economic time-series, alpha-stable distributions.

Organiser: Jean-Francois Emmenegger (Université de Fribourg, Switzerland)
Co-organiser: Elena Pervukhina (Sevastopol National Technical University, Ukraine)
Co-organiser: Tamara Bardadym (V.M.Glushkov Institute of Cybernetics, Ukraine)

The subject is situated in the domain of applied econometrics and economic time series analysis. Starting from actual economic questions arising in different countries the appropriate data and tools are set up. Thus, the proposed treated questions are as follows.

1) What quantity of given basic foods can a representative household or individual purchase with the earning power of its labour, represented by the mean monthly total wages, at any cross-sectional time point within a given period?
2) Is the consumer price index in equilibrium with mean total wages or with newly proposed price indices within a given period?
3) How to smooth and to forecast the prices of basic food in a given period with as less as possible a priori available information containing observational errors?
4) How do behave the returns of Eastern European Financial Markets since 1991?

The tools to analyse the questions are as follows.

1), 2) Cointegration analysis of economic time series, initiated by Engle and Granger (Nobel Prize in 2003), is the method to discover long-run equilibrium relationships between two or more analysed economic variables. Such analyses are of overall importance to verify equilibrium conjectures of economic theories.
3) An extension of the Kalman filter techniques used in state space time series filtering leading to adaptive filters, based on the minimisation of the Kullback–Leibler divergence criterion are proposed. Algorithms working under conditions of deficient information concerning the knowledge of the distribution of the error terms of the system are discussed.
4) The overall importance of α-stable distributions in opposition to the normal distribution to describe the returns' distributions is worked out. The Rachev-ratio and the STARR ratio as alternative to the Sharpe ratio are presented.

Parts of these subjects have been published in several papers like the International Journal of Applied Mathematics and in the WSEAS Transactions on Mathematics.

ARIMA, cointegration, Kalman-filter, alpha-stable distributions. **Jean-Francois Emmenegger** (Université de Fribourg, Switzerland) IC/MT683/008

Time-series econometrics has rapidly evolved in the last decades. Its progress is explained by its successful applications in macro- and micro-econometrics and especially by its rapid evolution in mathematical finance. The cointegration revolution has given great importance to this field, because linear cointegrating relations have economically interpretable coefficients, if they are related to questions of economics. Structural breaks have also got its methodology with Kalman filter applications as well as specific break detection algorithms. As economic theories also present time dependent dynamic problems, like the formation of capital intensity through the Solow equation, the mathematics of impulsive-difference equations has also been used to develop new solutions to these questions, cumulating to the impulsive Solow equation. The present international group around the project 'Analysis of Economic and Environmental Time Series', initiated since the 3rd ICIAM'95 in Hamburg, has worked in this field for more than 10 years and presents its theoretical results in terms of four fields of knowledge, probability, estimation, modelling and forecasting. But it has to be especially emphasised that this group has worked in this field with the aim to apply and combine the different mentioned modern methods of time series econometrics to practical subjects of real economy. Applications exist in the field of electricity consumption, purchasing power and consumer price index analyses, as well as dynamic modelling of capital intensity, Kalman filtering of price and ecological time series, but also the practical determination of alpha-stable distributions of index returns with the Fast

Fourier Transform Algorithm in empirical finance. These results are presented at this Minisymposium of the 6th ICIAM'07 in Zurich.

Cointegration applied to purchasing-power analysis of mean Ukrainian total wages. **Tamara Bardadym** (V.M.Glushkov Institute of Cybernetics, Ukraine), Jean-Francois Emmenegger (Université de Fribourg, Switzerland) IC/MT681/008

The main purpose of this paper is to propose a method of measurement of the purchasing power in Ukraine in approximately the last decade and to determine its evolution. Nineteen monthly price time series of basic food, the time series of the Consumer Price Index (CPI) and the Mean total Wages (MTW), published by the State Committee of Statistics of Ukraine (Derzhkomstat) have been selected within the period of November 1991 to December 2004. Preliminary studies of stationarity are undertaken to establish their degree of integratedness with a battery of adequate unit root tests. A cointegration analysis of couples of one of these price time series, respectively the CPI, and the MTW time series are undertaken within sub-periods of the interval 1991 to 2004, yielding linear functions between both selected time series, in order to establish tentative long-run equilibrium relations which are economically interpretable in terms of purchasing power analysis.

Adaptive time-series filters to smooth and forecast economic variables. **Elena Pervukhina** (Sevastopol National Technical University, Ukraine) IC/MT602/008

Classic filtering and prediction problems are solved on the basis of a differentiable matrix functional, defined on the coefficient matrix of the filter. The functional presents an information measure between the distribution parameters of the state vector and its tentative estimation and is well known as Kullback information divergence. The coefficient matrix provides the minimum of the functional and leads to a distribution for which the parameters are closest with respect to the distribution parameters of the real state vector of the system. Moreover, it needs only current observations of the system. The correspondent algorithm allows estimating the system state without a priori information on it and on the noise covariance, based on the observations. After data accumulation the filter acquires features closed to optimal filter characteristics. In particular, the norm of the covariance matrix of the estimation errors converges to the covariance matrix of errors after estimation of the optimal filter, using all the available a priori information. The numerical examples are connected with applied problems of smoothing and forecasting some ecological data from Crimea and some economic data from Ukraine with as less as possible available information on the noise of the system.

The stable Paretian hypothesis of Mandelbrot and the Gaussian hypothesis of Bachelier, ARMA and GARCH modelling for emerging Eastern European financial markets. **Anna Serbinenko** (Universität Karlsruhe, Germany) IC/MT4530/085

Bachelier (1900) had the path-breaking idea to model the returns of security and commodity markets as a random walk, meaning that successive differences of returns are Gaussian distributed. Despite of this fundamental idea, named the Gaussian hypothesis, Mandelbrot (1963) and Fama (1965) postulated that the distributions of the returns do not behave like this, but behave like the more general stable distributions, containing skewness and kurtosis. Mandelbrot called his concept the stable Paretian hypothesis. Rachev (2000) and other authors confirmed in their research work Mandelbrot's theses. Since then, a controversy between these both distributional hypotheses continue to exist in mathematical finance. Serbinenko and Emmenegger (2007) investigated the distributions of the returns of some financial market indices of the new emerging markets in Eastern Europe after 1991, confirming the stable Paretian hypothesis. Engle (1982) introduced the Autoregressive Conditional Heteroskedasticity (ARCH) model for the variance, and Bollerslev (1987) improved it by generalising the form of the model of the variance and developed the GARCH modelling technique. The present analysis follows these lines. The best fitted models of the returns of the financial market indices of these Eastern European countries are developed and validated, linear trend or ARMA(p,q) for the levels and GARCH(p', q') for the residuals. For risk evaluation financial indicators, the Sharpe-ratio (Gaussian hypothesis), the STARR- and the R-ratio (stable Paretian hypothesis) are calculated.

IC/MP586/013: Backward stochastic differential equations: simulations and applications.

Organiser: Emmanuel Gobet (INP Grenoble, France)

It is known that BSDEs have numerous applications and enable to solve some control problems in a random environment. The aim of this minisymposium is to bring together specialists of BSDEs, with in view different applications in physics, economics or finance.

Sequential Monte-Carlo methods to solve BSDEs. **Céline Labart** (Ecole Polytechnique, France), Emmanuel Gobet (INP Grenoble, France) IC/MT4356/013

Since 1990, the theory of BSDEs has been widely developed and it gives an alternative way to solve semi-linear PDEs. Numerical resolution is still a challenging task. Here we present an iterative approach, combining a Picard iteration and a sequential Monte Carlo approach.

Time discretization and Markovian iteration for coupled FBSDEs. **Christian Bender** (TU Braunschweig, Germany), Jianfeng Zhang (University of Southern California, USA) IC/MT4244/013

In this talk we propose a numerical algorithm to simulate high-dimensional coupled FBSDEs under weak coupling or monotonicity conditions. In particular we derive convergence of a time discretization and a Markovian iteration. The iteration differs from standard Picard iterations for FBSDEs in that the dimension of the underlying Markovian process does not increase with the number of iterations. This feature seems to be indispensable for an efficient iterative scheme from a numerical point of view. We finally suggest a fully explicit numerical algorithm and present some numerical examples with up to 10-dimensional state space.

An interpolated algorithm for quasi-linear PDEs. **Stéphane Menozzi** (University PARIS VII, France) IC/MT4939/088

We propose a time-space discretization scheme for quasi-linear parabolic PDEs. The algorithm relies on the theory of fully coupled Forward-Backward SDEs, which provides an efficient probabilistic representation of this type of equations. The derivated algorithm holds for strong solutions defined on any interval of arbitrary length.
The corner stone of the algorithm is a nonlinear quantized version of the dynamic programming principle. Then, the convergence analysis takes advantage of the standing regularity properties of the true solutionthrough an interpolation procedure and also exploits the optimality of the square Gaussian quantization used to approximate the conditional expectations involved.

In particular, our work provides an alternative to the method described in Douglas, Ma and Protter (Ann. Appl. Prob. 96) and weakens the regularity assumptions required in this reference as well as in the schemes introduced by Milstein and Tretyakov (see Stochastic Numerics for Math. Physics, Springer).

The stopping and starting problem in the model with jumps. **Said Hamadène** (Université Maine Le Mans, France) IC/MT4542/088

In this talk we focus on a real option problem namely the starting and stopping problem (or reversible investment) when the noise is driven by a Brownian motion and an independent Poisson process. This problem is tackled in using the notion of Snell envelope and Backward stochastic differential equations with jumps. We derive a stochastic verification theorem which we show later that is satisfied. When the random noise stems from a standard SDE with jumps we show that the problem is connected with a system of two variational inequalities. We finally give some numerical examples.

IC/MP115/008: Stochastic numerics: Monte-Carlo methods, SDEs, PDEs.

Organiser: Wesley Petersen (ETH Zürich, Switzerland)
Co-organiser: Michael Mascagni (Florida State University, USA)

Numerical simulations of stochastic differential equations of the form:

$$dX = b(X)dt + \sigma(X)dW$$

can be generalized to include stochastic partial differential equations (SPDEs) if the dimensionality of the process X is made large enough to resolve the coordinate space discretization. Topics in SDE simulations should include Ito SDEs (e.g. discontinuous drift coefficients), SPDEs, transport equations, high dimensional PDEs, and stochastic functional differential equations (delay equations). Other topics in this double minisymposium will include stochastic methods for potential problems.

Constrained stochastic differential equations in molecular dynamics. **Tony Lelièvre** (École Nationale des Ponts et Chaussées, France) IC/MT3482/088

We present some numerical schemes for SDEs with constraints. Such SDEs appear for example in kinetic modelling (rigid molecular bonds, computations at a fixed reaction coordinate value). After discussing the consistency of various numerical schemes, we more precisely discuss the sampling of Boltzmann-Gibbs measures on a sub-manifold by a gradient dynamics. We explain how such numerical schemes can be used to compute free energy differences in the NVT ensemble, or to sample the NVE ensemble.

Asset pricing in idiosyncratically incomplete markets: a numerical simulation. **Wesley Petersen** (ETH Zürich, Switzerland) IC/MT3512/088

In this ongoing work we consider the weak approximation of reflected Ito diffusions[2] using a projected Euler method. The goal is to compute $E[g(X_T) - \int_0^T h(X_t)\mathrm{d}\xi(t)]$ with a fixed time $T > 0$. This problem is related to the solution of parabolic PDEs with non-homogeneous Neuman boundary condition with value $h(x)$. Our current computations show an improvement in the weak order of convergence from $1/2$ to 1 for the mentioned projected Euler method. The main difficulty comes from approximating local time contributions at the reflection boundary.
Our main inspiration comes from the work[1], where weak order 1 has been achieved for the homogeneous Neuman boundary conditions case using a symmetrized Euler method.

[1] Bossy, M., Gobet, E. and Talay, D.; A symmetrized Euler scheme for an efficient approximation of reflected diffusions. J. Appl. Probab. 41, no. 3, (2004) pp.877–889.
[2] Freidlin, M.; Functional integration and partial differential equations. Annals of Mathematics Studies, 109.

Numerical methods for SDDEs with coloured noise. **Evelyn Buckwar** (TU Berlin, Germany) IC/MT3564/088

We consider stochastic delay differential equations with coloured driving noise. This type of equations appears, for example, in population dynamics. We develop and analyse numerical methods which are especially efficient for this type of equations. Numerical examples illustrate the numerical results.

Recent developments in the scalable parallel random-number generators (SPRNG) library. **Michael Mascagni** (Florida State University, USA), Wesley Petersen (ETH Zürich, Switzerland) IC/MT3653/088

This work presents the new and more versatile Scalable Parallel Random Number Generators Library (SPRNG). SPRNG is a widely used software package for both serial and parallel pseudorandom number generation. Its generators satisfy every known property of good pseudorandom numbers, and have passed some of the most stringent tests for pseudo-randomness available today. The previous versions of SPRNG used C as the implementation language and provided interfaces for FORTRAN and C++. Although SPRNG functions were callable from C++, the concepts of object-oriented programming were not applied in the implementation of earlier versions of SPRNG. In the new version, we replace the implementation language with object oriented C++, while still providing an interface for FORTRAN. Furthermore, we remove SPRNG's dependence on the GNU Multi Precision (GMP) Library and supplant GMP with our own accurate code for arithmetic on arbitrarily large integers and rational numbers. The resulting SPRNG library is as efficient as and complements the previous SPRNG versions and provides a wider user base access to high-quality parallel random number generation.The SPRNG library home page is http://sprng.fsu.edu.

IC/MP115/008: Stochastic numerics: Monte-Carlo methods, SDEs, PDEs. #2

Organiser: Wesley Petersen (ETH Zürich, Switzerland)
Co-organiser: Michael Mascagni (Florida State University, USA)

(For abstract, see session #1 above.)

Monte-Carlo methods for problems in biological electrostatics. **Michael Mascagni** (Florida State University, USA) IC/MT3654/088

We have been developing Monte Carlo methods for solving continuum electrostatic problems that arise in biochemistry. In vivo biochemistry takes place in ionic aqueous solution. When a molecule with fixed charges is places in such a solution, the free ions in the solvent reposition themselves accordingly. Accounting for the free ions can be done with explicit solvent models, such as molecular dynamics, or continuum models such as the nonlinear Poisson-Boltzmann equation. Previously we have developed methods for a linearized version of this problem; here we present new results on the full nonlinear Poisson-Boltzmann case.

Stochastic differential equations with discontinuous drift. **Sibylle Arnold** (ETH Zürich, Switzerland) IC/MT3331/008

New weak approximation schemes for SDEs $\mathrm{d}X_t = \mu(X_t)\mathrm{d}t + \sigma(X_t)\mathrm{d}B_t$, where B is a Brownian motion and the coefficients μ and σ are assumed to be only piecewise continuous, are presented. The new methods are based on an Exit problem approach and are shown by a statistical analysis to be superior to the Euler scheme for moderate stepsizes. The approach used for the statistical comparisons can be used in general to judge in a statistically significant way several weak approximation schemes regarding their goodness.

A fully-stochastic version of domain decomposition. **Maire Sylvain** (Université du Sud Toulon-Var, France) IC/MT3941/088

The standard way [1] to combine a deterministic method and the Monte Carlo method for domain decomposition is the following. The domain D is divided into two subdomains D_1 and D_2 separate by an artificial boundary $\Gamma_{1,2}$ An interpolation of the solution on $\Gamma_{1,2}$ is computed based on Monte Carlo approximations at some points of this boundary via the Feynman–Kac formula. Then the solution is computed on each subdomain by means of a deterministic method with the approximation on $\Gamma_{1,2}$ taken as a new boundary condition.The problem of this approach is that the error on the interface $\Gamma_{1,2}$ is usually large except if using a lot of trajectories with a small stepsize in the discretization scheme. We have introduced in [2] a new domain decomposition Monte Carlo algorithm to solve the Poisson equation in a domain D with Dirichlet boundary conditions where this problem is overcomed by using processes of correction and regularization at the interface. In this talk, we describe different strategies to optimize this method and its generalization to multidomain decomposition. Numerical simulations are given in the case of the Poisson equation over hypercubes.

[1] J. A. ACEBRON, M. P. BUSICO, P. LANUCARA, R. SPIGLER; Probabilistically induced domain decomposition method for elliptic boundary-value problems. Journal of Computational Physics, no.2, pp.421–438, 2005.
[2] E. GOBET, S. MAIRE; Sequential Monte Carlo domain decomposition for the Poisson equation, Proceedings of the 17 IMACS World Congress, Scientific Computation, Applied Mathematics and Simulation (2005).

Improving the stability of numerical simulations of quantum dynamical systems using stochastic differential-equation techniques. **Christian Perret** (ETH Zürich, Switzerland) IC/MT4052/088

Quantum dynamical systems typically deal with huge numbers of degrees of freedom, which makes them very difficult to simulate using deterministic methods. Modeling such systems with stochastic differential equations (SDEs) is an attractive option, but there remain stability problems. An example of a multi-dimensional complex SDE arises from an anharmonic oscillator with a one-mode BEC Hamiltonian given in [1], for which the numerical solution becomes unreliable after approximatively $t = 0.3$ for all tested numerical methods. Splitting of drift methods as introduced in [2] have been tried on this problem and improved the stability of the results, but not to the desired extent.

To improve the results, new numerical splitting methods have recently been developed. However, it seems that the choice of the numerical scheme alone might not guarantee the reliability of the results. The use of carefully chosen stochastic gauges as in [1] improves the accuracy of the simulation considerably by taking into account some aspects of the dynamics of the system, but so far the choices of gauges lead to a dissipative behavior of the diffusion part. The results using various techniques will be discussed.

[1] Deuar P., Drummond P.D.; Stochastic gauges in quantum dynamics for many-body simulations, Comput. Phys. Commun., 142 (2001), pp.442–445.
[2] Petersen, W.P.; A General Implicit Splitting for Stabilizing Numerical Simulations of Itô Stochastic Differential Equations, SIAM J. Numer. Anal., 35 (1998), pp.1439–1451.

IC/MP163/015: Probabilities meet scientific computing.

Organiser: Laurent Demanet (California Institute of Technology, USA)
Co-organiser: Lexing Ying (University of Texas at Austin, USA)

This workshop will overview recent research directions where probabilities help in designing efficient algorithms for intrinsically deterministic problems.

1) A first approach consists in randomly sampling rows and columns of a matrix, or apply the matrix to random vectors, in order to speed up the computation of low-rank approximations, like truncated SVD.
2) A second approach known as compressive sampling, or compressed sensing, consists in observing a signal in a *noise* basis in order to reconstruct it as a sparse superposition in another basis, by means of convex optimization techniques.
3) A third approach consists in modeling uncertainty about physical parameters through randomness, and solving for expectations and moments. This applies for instance to waves in random media.

Computational methods for waves in random media. **George Papanicolaou** (Stanford University, USA) IC/MT3209/015

The numerical simulation of wave propagation in random media is a challenge not only because we are typically interested in long distance propagation in media with inhomogeneities on many scales, but also because the usual notions of accuracy and computational complexity in the numerical solution of differential equations are not quite the right ones. The point is that since we model the medium by a random process, we do not know it in detail. We only know it statistically. In simulating wave propagation in such a medium we similarly do not want the waves calculated in all details, with numerical accu-

racy. We only want to compute them so that they have the correct statistical properties over long distances, and, if possible, with a simple method. I will address this problem and describe several methods that work well in different random media.

A randomized algorithm for the approximation of matrices. **Per-Gunnar Martinsson** (University of Colorado at Boulder, USA) IC/MT3210/015

In this talk, we will describe a randomized procedure for computing low-rank approximations to a given matrix. Specifically, suppose that we are given an $m \times n$ matrix A and a positive integer k, and that we seek to determine a matrix Z of rank k that approximates A (the matrix Z may be, *e.g.* a partial QR decomposition, or a partial singular value decomposition). The procedure that we propose solves the task by applying A and/or A^{t} to a sequence of l random vectors; it is particularly efficient whenever A or A^{t} can rapidly be applied to vectors (as happens, *e.g.*, when A is sparse, or is associated with the discretization of an integral operator). If l is only slightly larger than k, then the discrepancy between A and Z will be of the same order of magnitude as the $(k+1)^{\mathrm{st}}$ singular value σ_{k+1} of A with negligible probability of even moderately large deviations. As an example, we have proved that if $l = k + 20$, then the likelihood that the spectral norm $||A - Z||$ is greater than $10\sqrt{m(k+20)}\ \sigma_{k+1}$ is less than 10^{-17}.

We will describe applications of the scheme to numerical linear algebra, to signal processing, and to the design of fast algorithms for applying and inverting integral operators. We will also discuss techniques for how to adaptively determine the numerical rank of a given matrix. Several computational examples will be presented.

This is work done in collaboration with Vladimir Rokhlin and Mark Tygert.

Randomized algorithms for matrices, learning, optimization, and data. **Michael Mahoney** (Yahoo Research, USA) IC/MT3732/089

Much recent work in theoretical computer science, numerical linear algebra, machine learning, and statistical data analysis has exploited randomness as a computational resource to develop algorithms that provable approximate the solution to common matrix operations. Applications of such algorithms include the computation of low-rank matrix approximations qualitatively faster than traditional methods, sparsity-preservation in low-rank matrix approximations, speeding up kernel-based statistical learning, the efficient computation of coresets for common regression and optimization problems, and the improved scalability and interpretability of data analysis methods. We will describe recent algorithmic developments, with an emphasis on algorithms with provable *a priori* quality-of-approximation bounds. We will also discuss recent applications of this work to the scalable analysis of very large scientific and internet data sets.

Fast computation of Fourier integral operators. **Emmanuel Candès** (California Institute of Technology, USA), Lexing Ying (University of Texas at Austin, USA), Laurent Demanet (California Institute of Technology, USA) IC/MT4228/089

This talk introduces an efficient and novel algorithm for the numerical evaluation of Fourier integral operators (FIOs). This is of interest because FIOs are very important kinds of highly oscillatory integrals connected with wave propagation and which come up in a large number of applications. Examples in reflection seismology, radar imaging, ultrasound imaging, and electron microscopy all come to mind. Because an FIO is a dense matrix, a naive matrix vector product with an input given on a Cartesian grid of size N by N would require $O(N^4)$ operations. In contrast, our approach requires $O(N^{2.5}\log N)$ operations and as low as $O(N^{.5})$ in storage space (in practice, the constants are small). In numerical tests, the speedup factor over the naive evaluation for grids of size 512 by 512 is close to 200.

The algorithm operates by localizing the integral over polar wedges with small angular aperture in the frequency plane. On each wedge, the algorithm factorizes the highly oscillatory kernel into two components: 1) a diffeomorphism which is handled by means of a nonuniform FFT and 2) a residual factor which is handled by numerical separation of the spatial and frequency variables. In some sense, the algorithm can be seen as a generalization of the FFT for inhomogeneous phases and amplitudes. We also demonstrate the numerical accuracy and low computational complexity of the proposed methodology.

This is joint work with Laurent Demanet and Lexing Ying.

08: Probability and Statistics, Contributed Talks

IC/CTS4684/08: **Statistics.**

Organiser: Shariful Alam (Department of Mathematics, Bengal Engineering and, India)

Optimal sequential decision-rules with restrictions. **Vadim Arkin** (Russian Academy of Sciences, Moscow) IC/CT957/010

We obtain necessary and sufficient optimality conditions for general stopping problems with terminal decisions and integral restrictions. These problems are connected with sequential analysis and some aspects of financial mathematics. In particular, for the case of several hypotheses about the observable process the problem under discussion can be reduced to Bayesian one with Lagrangian as a risk function.

Let $(\Omega, \mathcal{F}_t, \mathcal{F}, \mathbf{P})$ be a standard stochastic basis, $\mathcal{P}$ be a σ-algebra of progressively measurable sets, and $\mathcal{M}$ be a class of stopping times respect to $\mathcal{F}_t$. A pair $\delta = (\tau, d_\tau)$ will be called a decision rule if $\tau \in \mathcal{M}$, and d_τ be $\mathcal{F}_\tau$-measurable function with values in a complete separable metric space $(D, \mathcal{D})$.

Let $\mathcal{D} \times \mathcal{P}$-measurable functions $\varphi_0(d,t,\omega), \ldots, \varphi_n(d,t,\omega)$ and non-empty set $Q \in \mathcal{D}$ are given. Consider the following extremal problem:

$$\Phi_0(\delta) = \mathbf{E}\,\varphi_0(d_\tau, \tau) \to \max_\delta,$$
$$\Phi_i(\delta) = \mathbf{E}\,\varphi_i(d_\tau, \tau) \le 0, \quad i = \overline{1,n}, \quad d_\tau(\omega) \in Q,\ \mathbf{P}-\text{a.s.}$$

Denote $H(d,\tau) = \varphi_0(d,\tau) - \sum_{i=1}^n \Lambda_i \varphi_i(d,\tau)$.

Theorem *Let σ-algebra $\mathcal{F}_0$ does not contain $\mathbf{P}$-atoms, $\Phi_0(\delta^*) < \infty$, and there exists $\hat{\delta}$ such that $\Phi_i(\hat{\delta}) < 0$, $i = \overline{1,n}$. Then decision rule $\delta^* = (\tau^*, d^*_{\tau^*})$ be optimal if and only if there exist values $\Lambda_i \ge 0$, $i = \overline{1,n}$ such that*

1. $\tau^* = \operatorname{argmax}_{\tau \in \mathcal{M}} \mathbf{E} \sup_{d \in Q} H(d,\tau)$;
2. $d^*_{\tau^*} = \operatorname{argmax}_{d \in Q} H(d, \tau^*) \quad (\mathbf{P}-a.s.)$,
3. $\sum_{i=1}^n \Lambda_i \mathbf{E}\,\varphi_i(d^*_{\tau^*}, \tau^*) = 0$.

Multivariate Poisson summation formula applied to estimation of closeness to the uniform distribution. **Vladimir Khokhlov** (Steklov Mathematical Institute, Russian Federation) IC/CT506/010

A probabilistic interpretation of the multivariate Poisson summation formula (PSF) gives a way to estimate the deviation $\Delta = \sup_{\mathbf{x}_{(s)}\in[0,1]^s} |\, p\,(\mathbf{x}_{(s)};\{\mathbf{X}_{(s)}\}) - 1\,|$ of the density $p\,(\mathbf{x}_{(s)};\{\mathbf{X}_{(s)}\})$ of the distribution of a random vector $\{\mathbf{X}_{(s)}\}$ consisting of components which are fractional parts of components of a random s-dimensional vector $\mathbf{X}_{(s)}$ in $\mathbb{R}^s$ from the density of the uniform distribution in the unit s-dimensional cube $[0,\,1]^s$ in $\mathbb{R}^s$.

Under some conditions which make it possible to apply PSF, we get the upper bound $\Delta = \sup_{\mathbf{x}_{(16)}\in[0,1]^{16}} |\, p\,(\mathbf{x}_{(16)};\{\eta\,\mathbf{Z}_{(16)}\}) - 1\,| \;\le\; \dfrac{P(q)}{(1-q)^8}$ for the vector $\{\eta\,\mathbf{Z}_{(16)}\}$ of fractional parts of the random Gaussian vector $\eta\,\mathbf{Z}_{(16)}$ having a nonsingular covariance matrix; $P(q)$ is a polynomial of the seventh degree of $q = e^{-2\pi^2\eta^2\lambda}$; where $\eta > 0$ is an arbitrary scaling parameter, which may increase infinitely in applications, and $\lambda > 0$ is the minimal eigenvalue of the covariance matrix. The proof is based on the upper bound for the number $r_{16}(N)$ of integer points $\mathbf{m}_{(16)} = (m_1, m_2, \ldots, m_{16}), m_\nu \in \mathbb{Z}$, lying on the 16-dimensional sphere $S_{16}(\sqrt{N})$, for $N \in \mathbb{Z}^+$. The approach can be extended to higher dimensions s, being a multiple of 16 (see[1]).

[1] Khokhlov, V.I.; A method of estimation of the number of integer points on the multidimensional sphere and its application to the problem of estimation of closeness to the uniform distribution. Obozr. Prikl. Prom. Mat. **13** (2006), pp.3–27.

Asymptotics of the log*-partition function and new algorithms for counting without sampling.* **Antar Bandyopadhyay** (Indian Statistical Institute (Delhi Centre)), David Gamarnik (Massachusetts Institute of Technology, USA) IC/CT4327/082

In this talk we will propose new methods for computing the asymptotic value for the logarithm of the partition function for certain statistical physics models on certain type of finite graphs, as the size of the underlying graph goes to infinity. We will consider two models, namely the *hard-core* model when the *activity* parameter λ is *small*, and the model for counting the number of proper q-colorings. And we will only consider the graphs with *large girth*. In particular, we will show that asymptotically the logarithm of the number of *independent sets* of any r-regular graph with large girth is constant, when $r \le 5$. For example, we will show that every 4-regular n-node graph with large girth has approximately $(1.494...)^n$-many independent sets, for large n. Similarly we will prove that for every r-regular graph with $r \ge 2$, with n nodes and large girth, the number of proper $q \ge r+1$ colorings is approximately a constant (which can be explicitly written in terms of q and r), when n is large. Similar results also hold for random regular graphs. As a byproduct of our method we will show that one can obtain some simple approximate counting algorithms for the problem of enumerating the number of independent sets, and proper colorings, in low degree graphs with large girth. These algorithms will be deterministic as opposed to Markov chain sampling schemes which are typically used in this context. Our main approach will be to use a (strong) *correlation decay* property for the corresponding Gibbs measure (at certain parameter regime), along with a simple *cavity trick* which is well known in the physics literature.

Time-series modelling of the Singapore population data. **Wai Kwong Cheang** (Nanyang Technological University, Singapore) IC/CT1813/085

Trends in population have important implications for a government in formulating its manpower-related policies. A business may also need to adjust its long-term market strategies according to these trends. This paper analyses the Singapore population data using time series regression model with autoregressive error term. In addition to a linear trend, other regressors included in the model are (i) a seasonal component of period 12 to account for the effect of the auspicious "dragon" years in the Chinese calendar; (ii) level-shift interventions to account for the effect of the government campaigns on family planning. Two methods of estimating the autoregressive parameter are considered: maximum likelihood (ML) and restricted maximum likelihood (REML). For a time series of short or moderate sample length, it is shown in Cheang and Reinsel (2000) [Bias reduction of autoregressive estimates in time series regression model through restricted maximum likelihood, Journal of the American Statistical Association, 95, 1173–1184] that the REML estimator is generally much less biased than the ML estimator. This paper compares the ML and REML estimation results, and examines the implications for the nature of nonstationarity (deterministic or stochastic trend component) exhibited by the Singapore population data series.

Prediction of bond ratings using statistical and neural network techniques. **Shariful Alam** (Department of Mathematics, Bengal Engineering and, India) IC/CT4243/008

Quantitative models have been developed to predict bond ratings of firms in the Indian Manufacturing Sector, using Financial Leverage, Profitability, Asset Management Ability, Stability and Market Sensitivity of the firm, which totally involved 16 variables. These 16 independent variables are first reduced to seven orthogonal variables using Principal Component Analysis. Then these variables are used to build three types of quantitative models namely Multiple Discriminant Analysis (MDA) model, Multinomial Logistic Regression (MLR) model and Artificial Neural Networks (ANN) model.

MDA models are developed using two approaches, viz., FisherŠs Discriminant Analysis (FDA) and Discriminant Analysis by MLE method [Quadratic Discriminant Analysis (QDA)]. Comparison is made between FDA and QDA models and it is found that QDA model is superior to FDA model. In MLR attempts have been made to build proportional odds model and subsequently conventional full multinomial logit model. It is found that the proportionality of odds is violated and an appropriate multinomial logit model is proposed. In ANN a feed forward neural network with one hidden layer is chosen for analysis. Network size and geometry is finalized after experimenting with 5 logically built networks. Levenberg-Marquardt BP algorithm is used as the training algorithm and MSE (mean squared error) is used as network performance function during training. After some trial and error, Tan-Sigmoid (tansin) is used in the hidden node and Log-Sigmoid (logsin) is used in the output node as activation functions.

Based on both in-sample classification and out-sample validation it is found that both MLR and ANN models are superior to MDA, with little difference in performance between themselves.

On the stability of some stochastic integral equation. **Khairia El-Nadi** (Alexandria University, Egypt) IC/CT24/010

Stochastic Volterra equations of the form:

$$dx(t) = f(x(t))dt + \int_0^t K(t-s)x(s)ds\;dt + g(x(t))dB(t),$$

are considered, where $\{B(t) : t \ge 0\}$ is standard one-dimensional Brownian motion and the kernel K decreases to zero non-exponentially. We study the convergence rate to zero of the stochastic solutions of the considered equation. It is

proved under suitable conditions that :

$$\lim_{t\to\infty} \frac{|x(t)|}{K(t)} = \infty, \quad \text{almost surely.}$$

The considered stochastic integral equations arise if we consider the Black–Scholes market consists of a Bank account or a bond and a stock. These stochastic models can also be applied to population dynamics in biology.

IC/CTS4686/08: Networks, queues.

Organiser: Stephane Chretien (Université de Franche-Comté, France)

Reliability enhancement and fixed transmission times of acyclic transmission multiŰstate networks (ATMNs). **Sanjay Chaudhary** (Ambedkar University, Agra, India) IC/CT761/010

In this talk, an algorithm for acyclic transmission multi-state networks (ATMNs) is suggested in which each network has a root position where the signal source is located, a number of leaf (terminal) nodes that can only receive the signal, and a number of non-leaf (non-terminal) nodes that retransmit the received signal to some other nodes. The signal propagation from root node to terminal nodes, which avoid the cycle. The time of the signal transmission between each pair of nodes in ATMNs depends on the type of equipment and exchange protocols. Two types of networks are considered in which one type network has individual multi-state elements (MEs) located at different positions. Second type networks have two MEs located at same position and other MEs located at different positions individually. The universal generating function technique is applied in ATMNs for evaluating the system reliability and expected value in specified time.

On a queueing system that exhibits Markovian character due to service interruptions. **A Krishnamoorthy Krishnamoorthy** (Cochin University, India) IC/CT2829/082

We consider a service system which exhibits a kind of Markovian property momentarily if and when the Markovian property is revealed due to a service interruption, the service is repeated. On the other hand if the service interruption does not result in the realization of the Markovian property, the current service is resumed. We analyse the system under very general assumptions on interarrival, service time and repair time (due to interruption) distributions. These are assumed to be independent of each other. Several performance measures are obtained. Some numerical results are provided. This model finds applications in medicine, in certain manufacturing processes with interruption, and certain learning processes.

Risk-constrained scheduling of electricity markets. **Arash Ehsani** (Islamic Azad University, Iran), AliMohammad Ranjbar (Sharif University of Technology, Iran), Mahmud Fotuhi-Firuzabad (Sharif University of Technology, Iran) IC/CT2842/008

Electricity markets are typically operated at least cost subject to technical constraints. This paper presents a probabilistic model for competitive electricity markets. A competitive structure is proposed which includes a purchasing agency with centrally optimized scheduling. Supply reserve is considered in the proposed approach. The value of risk is deduced from the supply model. The required supply model is constructed using the outage replacement rate (ORR) of energy production units. On demand side, the consumption forecast uncertainty is included. The performance of the proposed method is verified through numerical case studies.

Complete coverage and eventual coverage of space by random sets. **Anish Sarkar** (ISI Delhi, India) IC/CT1408/082

We consider of a point process on S on a subset of $\mathbb{R}^d$ for $d \geq 1$. With each point of the point process, we associate a random shape (we consider only sphere with i.i.d. radius and squares with i.i.d. side lengths here). Let C be the random region covered by these random shapes. We are interested in some coverage properties of this random set C. If $S = \mathbb{R}^d$, the main question that one asks, is about complete coverage; i.e., under what conditions is $C = \mathbb{R}^d$? (see Hall [1988] and Meester & Roy [1996]). Athreya et. al. [2004] introduced the notion of eventually coverage, where they studied the properties of C when $S = (0,\infty)^d$ when the underlying point process is a homogeneous Poisson process in $d = 1$ or $d \geq 2$. We extend these concepts for the half-spaces and study the eventual coverage of certain unbounded sets of the half-space. We show that the eventual coverage depends on the tail behaviour of the radius random variable.

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An SDP relaxation of the sparsest recovery problem. **Stephane Chretien** (Université de Franche-Comté, France) IC/CT3182/088

The problem of recovery of the sparsest solutions to overdetermined linear systems of equations has recently been addressed by several authors starting with Candès, Romberg and Tao [E. J. Candès, J. Romberg and T. Tao (2004). Robust Uncertainty Principles: Exact Signal Reconstruction from Highly Incomplete Frequency Information, IEEE Inf. Theory 52 (2006) Vol 2., 489–509]. This problem is of great theoretical as well as practical importance. Indeed, looking for sparse representation of information is a new way to look at various fields such as modern harmonic analysis, numerical approaches to PDE and statistics with wide ranging scope of applications.

One of the breaktroughs in the work of Candes, Romberg and Tao was the realization that the $\mathcal{NP}$-hard optimization problem of finding the sparsest solution to overdetermined linear systems of equation can be solved with high probability using linear programming (LP) via a simple substitution of the sparsity objective function with values in $\mathbb{N}$ with the l_1 norm of the vector to be optimized. Formally, for any vector $x \in \mathbb{N}$, let $\|x\|_0$ denote the number of nonzero components of x and let $\|x\|_1$ denote its l_1 norm that is the sum of the absolute values of its components. The problem of finding the sparsest solution to the system

$$Ax = b \tag{1}$$

with A in $\mathbb{R}^{m\times n}$, b in $\mathbb{R}^m$ and m much smaller that n can be written as the following optimization problem

$$\min_{x\in\mathbb{R}^n} \|x\|_0 \text{ s.t. } Ax = b. \tag{2}$$

The convex relaxation is given by

$$\min_{x\in\mathbb{R}^n} \|x\|_1 \text{ s.t. } Ax = b \tag{3}$$

and can easily transformed into a linear program.

The goal of this paper is to present a stronger convex relaxation using semidefinite programming (SDP) for which efficient interior point method have been designed and various packages exist such as SeDuMi for Matlab. This class of convex optimization problems has been the subject of an intense research activity in the nonlinear optimization community, leading to efficient polynomial time algorithms for various difficult problems in combinatorics and engineering; see for instance [Nemirovski, A. Advances in Convex Optimization: Conic Programming - to appear in Volume I (Plenary Lectures) of International Congress of Mathematicians, Madrid 2006, European Mathematical Society, 2006].

The strengthened relaxation we propose is obtained as follows. Introduce the vector $z \in \mathbb{R}^n$ of 0-1 variables. This vector will index the components of x which should be set to zero through the constraint

$$z^t x = 0 \tag{4}$$

Now the cost function is given by $\sum_{i=1}^{n} z_i$ which is exactly the number of components of x equal to zero. The constraints specifying the binary nature of z are of the form

$$z_i(z_i - 1) = 0 \text{ for } i = 1, \ldots, n. \tag{5}$$

To sum up, we obtain a new representation of the sparsest recovery problem, given in the form of a quadratically constrained nonconvex optimization problem as

$$\begin{array}{l} \max_{x,z \in \mathbb{R}^n} e^t z \\ texts.t. \left\{ z_i(z_i - 1) = 0, \quad i = 1, \ldots, n \quad z_i x_i = 0, \quad i = 1, \ldots, n \quad Ax = b. \right. \end{array} \tag{6}$$

As is well known in the optimization community, the class of quadratically constrained quadratic programs to which this problem belongs, admits SDP relaxations. SDP are convex optimization problems over the cone of positive semidefinite matrices in the set of real symmetric matrices. This relaxation can be obtained in a systematic manner using Lagrangian duality, leading in the present case to a problem of the form

$$\begin{array}{l} \max_{X \in \mathbb{S}_{2n+1}} \operatorname{trace}(A_0 X) \\ texts.t. \left\{ \operatorname{trace}(A_j X) = c_j, \quad i = 1, \ldots, m + 2n + 1 \quad X \succeq 0. \right. \end{array} \tag{7}$$

where $\mathbb{S}_n$ is the set of real symmetric matrices of order n and $A \succeq B$ is the order relation generated by the cone of positive semidefinite matrices.

We will show in particular that this relaxation is stronger than the previous one and provide simulations results proving the applicability of this new approach.

Scale's descriptions, system's approach to risks. **Natalia Serdyukova** (Academy of Budget and Treasury, Russian Federation) IC/CT4811/071

Full classification of all types of scales is obtained in terms of group of admissible transformations of scale. Matrix, lattice, and multidimensional scales are introduced. It is proved that twodimensional scales are the most informative. Lump-sum function of risk is defined in probability space as dual function to probability measure. Owing to common dual theory constructed function repels the most common typical behaviour of risk. Some wellknown measuring instruments, such as generalize dispersion satisfy to proposed scheme.

IC/CTS4687/08: Applied probability, I.

Organiser: Tim Heaton (University of Oxford, UK)

Investigation of properties of the solutions of hyperbolic SPDE. **Oleksiy Ignatyev** (Institute of Apllied Mathematics and Mechanics of, Ukraine) IC/CT709/082

We consider the space-time white noise-driven stochastic partial differential equation (SPDE) on $R_T = [0,T] \times [0,+\infty)$.

$$\frac{\partial^2 u(t,x)}{\partial t \partial x} = u^{\alpha}(t,x) \quad \frac{\partial^2 W(t,x)}{\partial t \partial x}$$

$$u(0,x) = \tilde{u}(x), \qquad u(t,0) = p(t)$$

where $T > 0$ is fixed but arbitrary. $W(t,x)$ is the Brownian sheet corresponding to the driving space-time white noise-with intensity Lebesgue measure-written formally as $\partial^2 W / \partial t \partial x$. The functions $\tilde{u}(x)$ and $p(t)$ are taken to be continuous bounded deterministic functions.

In this paper we investigate whether the solution $u(t,x)$ of the above hyperbolic SPDE has compact support property for all $t > 0$ providing that $\tilde{u}(x)$ has compact support property.

Branching principal components, principal cubic complexes and topological grammars. **Alexander Gorban** (University of Leicester, UK), Andrei Zinovyev (Institut Curie, France), Neil Sumner (University of Leicester, UK) IC/CT1269/087

A method of topological grammars is proposed for multidimensional data approximation. For data with complex topology we define a principal cubic complex of low dimension and given complexity that gives the best approximation for the dataset. This complex is a generalization of linear and non-linear principal manifolds and includes them as a particular case. The problem of optimal principal complex construction is transformed into a series of minimization problems for quadratic functionals. These quadratic functionals have a physically transparent interpretation in terms of elastic energy. For the energy computation, the whole complex is presented as a system of nodes and springs. Topologically, the principal complex is a product of one-dimensional continuums (represented by graphs), and the graph grammar [1] describes transformation of these factors during construction of the optimal complex. This factorization of the whole process onto one-dimensional transformations and using minimization of quadratic energy functionals allow us to construct efficient algorithms. The topology of the complex is not prescribed, but adaptive. In that sense, they are even more flexible than SOMs [2]. The whole approach can be interpreted as an intermediate between very flexible neural gas and significantly more restrictive elastic maps [3]. It includes as simple limit cases the k-means clustering algorithm, classical PCA and Principal manifolds [4].

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Stable computation of probability densities for metastable dynamical systems. **Susanna Kube** (Zuse-Institut Berlin, Germany), Marcus Weber (Zuse-Institut Berlin, Germany), Peter Deuflhard (Zuse-Institut Berlin, Germany) IC/CT3976/088

Whenever the invariant stationary density of metastable dynamical systems decomposes into almost invariant partial densities, its computation as eigenvector of some transition probability matrix is an ill-conditioned problem. In order to avoid this computational difficulty, we suggest to apply an aggregation/disaggregation method which only addresses well-conditioned sub-problems and thus results in a stable algorithm. In contrast to existing methods, the aggregation step is done via a sampling algorithm which covers only small patches of the sampling space. We will show how this method allows the correct computation of statistical weights for molecular conformations.

Weak predictor–corrector schemes for jump diffusions. **Nicola Bruti Liberati** (University of Technology, Sydney, Australia), Eckhard Platen (University of Technology, Sydney, Australia) IC/CT714/088

Event-driven uncertainties such as corporate defaults, operational failures or central bank announcements are important elements in the modelling of financial quantities. Therefore, stochastic differential equations (SDEs) of jump-diffusion type are often used in finance. We consider in this paper weak discrete time approximations of jump-diffusion SDEs which are appropriate for problems such as the evaluation of moments, derivative prices, risk measures and expected utilities. We present regular and jump-adapted predictor-corrector schemes with first and second order of weak convergence. The regular schemes are constructed on time discretizations that do not include jump times, while the jump-adapted schemes are based on time discretizations that include all jump times. Finally, we test the accuracy of these schemes when applied to the jump-diffusion Merton model.

Bivariate geometric models and their applications. **Jayakumar Kuttan Pillai** (University of Calicut, India) IC/CT2858/008

Geometric distribution possess lack of memory property and is applied in a variety of contexts. Characterizations of a bivariate geometric distribution using univariate and bivariate geometric compounding are obtained. Autoregressive models with marginals as bivariate geometric distribution are developed. Various bivariate geometric models analogous to important bivariate exponential distributions like, Marshall–Olkin bivariate exponential, Downton's bivariate exponential and Hawkes' bivariate exponential are introduced and studied.

Discrete Mittag–Leffler distribution is a class of distributions containing geometric distribution. Discrete Mittag–Leffler distribution is infinitely divisible and is normally attracted to stable law. In this paper various bivariate discrete Mittag–Leffler models are introduced. Various characterizations of discrete Mittag–Leffler distributions are obtained through closure under geometric summation and repeated geometric summation. Time sreies models with bivariate discrete Mittag–Leffler marginals are developed and their properties are studied.

Key words:- Autoregressive process, Bivariate exponential distribution, Bivariate geometric distribution, Characterization, Compounding.

IC/CTS4685/08: Probability.

Organiser: Sheldon Jacobson (Univ. of Illinois at Urbana-Champaign, USA)

Some results on generalised probability-distribution functions. **Rajendra Kumbhat** (Jai Narain Vyas University, India), Shanu Sharma (Jodhpur, India) IC/CT3251/010

In this paper a generalised probability distribution function has been introduced using generalised hypergeometric function 2R1(.) from which almost all classical probability distribution functions defined earlier can be obtained as special cases.For the probability distribution function,the moment generating function,moments and the characterstic functions have been investigated.The distribution of linear combination of independent variables has also been worked out. Kindly acknowledge the receipt.

On the accuracy of the normal approximation to the distributions of Poisson random sums. **Irina Shevtsova** (Moscow State University, Russian Federation) IC/CT1097/010

Let $X_1, X_2, \ldots$ be a sequence of independent identically distributed random variables with finite moments of order $2+\delta$ with some $\delta \in (0,\,1]$ and N_λ be a Poisson random variable with parameter $\lambda > 0$, independent of $X_1, X_2, \ldots$ for each $\lambda > 0$. Denote $F_\lambda(x)$ the distribution function of the standardized Poisson random sum $X_1 + \ldots + X_{N_\lambda}$ and $\Phi(x)$ the standard normal distribution function. We show that under above assumptions the following analogue of the Berry–Esseen inequality holds:

$$\rho(F_\lambda,\,\Phi) \equiv \sup_x |F_\lambda(x) - \Phi(x)| \le \begin{cases} C(\delta)\cdot L_\lambda^{2+\delta}, & \text{for } 0<\delta<1, \\ 0.7056\cdot L_\lambda^3, & \text{for } \delta = 1, \end{cases}$$

where $L_\lambda^{2+\delta}$ is the noncentral Lyapunov fraction and

$$C(\delta) = \frac{2^{1-\delta/2}\Gamma(\frac{2+\delta}{2})}{\pi(1+\delta)(2+\delta)}.$$

As it can easily be seen, the function $C(\delta)$ monotonically decreases varying within the range $(6\sqrt{2\pi})^{-1} = C(1-) \le C(\delta) \le C(0+) = \pi^{-1}$.

We also show that for $\delta = 1$ under additional assumption of integrability of the characteristic function of the random summands the following refined estimate holds:

$$\rho(F_\lambda,\Phi) \le \frac{L_\lambda^3}{6\sqrt{2\pi}} + O\Big(\frac{\sqrt{\ln\lambda}}{\lambda}\Big),$$

given an explicit expression for the latest term.

Correcting the Monte-Carlo optimal-stopping bias. **Tyson Whitehead** (University of Western Ontario, Canada), Matt Davison (University of Western Ontario, Canada), Mark Reesor (University of Western Ontario, Canada) IC/CT4512/086

Optimal-stopping problems are frequently solved by approximating them as discrete optimal-stopping problems, and then applying Bellman's principle to break them up into a series of sub-problems to be solved via Monte Carlo and then optimally recombined. The problem with this is that, while each sub-problem may be evaluated in a non-biased manner, the process of recombination favours those sub-problems whose value has been overestimated, introducing solution bias. We present an overview of our asymptotic work showing how to derive a first-order correction term for this effect. We also present the results of applying such a correction term to the stochastic-mesh technique in a financial example, a well-studied multivariate pricing problem, which demonstrates the resulting significant computational advantage.

Stochastic homogenization on self-similar structures. **Anna Soos** (Universitatea Babeş-Bolyai, Romania) IC/CT908/082

The homogenization theory is devoted to analysis of partial differential equations with rapidly oscillating coefficients. Let $\mathcal{A}^k$ be a given partial differential operator and we consider the equation $\mathcal{A}^k u^k = f$, together with the appropriate boundary initial conditions. Here $k \in \mathbb{N}$ and $f \in H^1(\mathbb{R}^n)$. We are interested in studying the solutions of this system in the limit as $k \to \infty$. The homogenization theory study the convergence of u^k, as $k \to \infty$, characterize the limiting process and construct the limiting equation. In this article we will quit the periodicity assumption. The coefficients are generated by an iterated function system. We will give a new kind of homogenization method on selfsimilar structures. We will use some basic notions from the fractal geometry as the invariant set and invariant measure of an iterating function systems.

The economic impact of obesity on automobile fuel consumption in the United States. **Sheldon Jacobson** (Univ. of Illinois at Urbana-Champaign, USA) IC/CT2484/010

Obesity has become a major public health problem in the United States. There are numerous health implications and risks associated with obesity. One socio-economic implication of obesity is that it reduces passenger vehicle fuel economy (i.e., the miles per gallon achieved by automobiles, which include cars and light trucks driven for noncommercial purposes). This paper quantifies the amount of additional fuel consumed (annually) in the United States by automobiles that is attributable to higher average passenger (driver and non-driver) weights, during the period from 1960 to 2002. The analysis uses existing driving data in conjunction with historical weight data. The results indicate that, since 1988, no less than 272 million additional gallons of fuel are consumed annually due to average passenger weight increases. This number grows to approximately 938 million gallons of fuel when measured from 1960, which corresponds to approximately 0.7% of the nation's annual fuel consumption, or almost three days of fuel consumption by automobiles. Moreover, more than 39 million gallons of fuel are estimated to be used annually for each additional pound of average passenger weight. This research is co-authored with Laura A. McLay.

A stochastic interpretation of the Mumford–Shah functional. **Tapio Helin** (Teknillinen Korkeakoulu, Finland) IC/CT2710/085

Inverse problems are related to solving quantities that cannot be measured directly. A typical property of inverse problems is their ill-posedness. In Bayesian inversion theory the problem is formulated as a statistical inference problem based on stochastic models of indirect measurements and *a priori* information. In this setting the solution is the posterior probability distribution.

In 1989 Mumford and Shah proposed their celebrated minimization method for image segmentation. The method combines shape and functional minimization thus making the computational problem challenging.

In this talk we discuss the connections between the Mumford-Shah –functional and the Bayesian approach in statistical inverse problems.

This work has been done in collabration with Professor Matti Lassas, Helsinki University of Technology, Finland.

IC/CTS4688/08: Applied probability, II.

Organiser: Nicole Marheineke (TU Kaiserslautern, Germany)

Symbolic–numeric algorithms for analysis of stochastic systems with different forms of after-effect. **Igor Poloskov** (Perm State University, Russian Federation) IC/CT783/088

An analysis of random phenomena in dynamic systems of various types is a very important subject both for theory and practice. The necessity of such analysis is urgent for study of different events: (i) a flight of vehicles under an action of atmospheric turbulence; (ii) a traffic along a rough road; (iii) high-altitude vibrations of structures under wind and seismic attacks etc.

Effects of delay in different forms occur in a lot of tasks. Such phenomena appear, where features of objects are defined by an action of aftereffect, for example there are processes of automatic control for technical devices and engineering procedures, economic and social systems, struggle of species for existence in biology and so forth.

The main idea of our technique for stochastic differential equations with single and multiple, constant and variable delays is to expand the phase space of appropriate system and to reduce a non-Markovian vector process to a Markovian one. By this way we construct:

– chains of Fokker-Planck-Kolmogorov-like equations satisfied by the (transitional) probability density functions for vectors belonging to a family of embedded phase spaces;

– chains of equations for moments of these vectors.

Further we define a number of stochastic cases for a classic method of steps and demonstrate an exploitation of the cumulant closure for nonlinear systems at a stage of numerical calculations on the base of our Mathematica-code package ProbRel.

The idea of the phase extension is used for study of linear stochastic integro-differential equations with additive and multiplicative noises.

The techniques are applied to study a number of linear and nonlinear models such as linear equations of car motion effected by front-to-rear delay and a rough road; dynamics of pollutions discharged into a cascade of natural water bodies; a nonlinear system with multiple delays; a Black-Scholes model with a constant delay and Wiener and Poisson random excitations etc.

Spherical codes: separation, discrepancy and energy. **Paul Leopardi** (Australian National University) IC/CT1125/088

On the unit sphere $S^d \in \mathbb{R}^{d+1}$, a construction is given for a spherical code called the EQ code. The sequence of EQ codes is well separated.

For $0 < s < d$ a sequence of S^d codes which is well separated and weak star convergent has a Riesz s energy which converges to the corresponding energy double integral. A bound is given on the rate of convergence of Riesz s energy given the rate of convergence to zero of the spherical cap discrepancy.

Estimates are given for the rate of convergence to zero of the spherical cap discrepancy of the EQ codes, and the rate of convergence of the Riesz s energy of the EQ codes to the energy double integral.

Stochastic model for fiber lay-down process in non-woven production. **Nicole Marheineke** (TU Kaiserslautern, Germany) IC/CT4016/008

In this work a stochastic model for the lay-down of fibers on a conveyor belt in the production process of nonwovens is presented and investigated. The model is based on a stochastic differential equation taking into account the fiber dynamics under the influence of turbulence. A reformulation as a stochastic Hamiltonian system and an application of the stochastic averaging theorem lead to further simplifications of the model. The model is used to compute the distribution of process functionals that might be helpful for the quality assessment of industrial fabrics.

Adaptive detection of distribution changes in a medical information system. **Jack Xue** (Butler Univ. & Conseco Insurance, USA) IC/CT22/010

As a delivery engine of the Regenstrief Medical Recording System (RMRS), the web-based medical document distribution system, Docs4Docs™, is used by thousands physicians in hundreds practices in Indianapolis area to receive laboratory reports, medical transcriptions and patient admission/discharge reports[1]. Docs4Docs collects these critical medical documents as HL7 messages via RMRS and process them into hospital-approved printable format and deliver them to practices' document inbox within a given amount of time. To fulfill the latency requirement, it is critical for Docs4Docs to receive these HL7s in time. Supposing that the latency owing to the HL7 message receiver (receiver, for short) is negligible, the latency in delivery then solely depends on access, transportation and storage of these HL7s along the uploading path.

The Statistical Process Control (SPC) methods, such as p-chart, has been used to monitor the process performance, such as pharmacy expert systems[5]. However, it has been proved that the Sequential Probability Ratio Tests (SPRT), which is the foundation of our algorithm is a superior surveillance tool because it is sensitive not only to disturbances in the signal mean, but also to very subtle changes in the statistical quality (variance, skewness, bias) of signals[4]. Wald[6] proved the optimality of SPRT in case that all random variables in the sequence are independent and identically distributed (i.i.d.) in 1947. Basseville and Nikiforov[7] formulated the fault detection problem as a stochastic dynamic system in 1993. Siegmund and Venkatraman[8] proved the statistical properties of this system in 1995. Lai[9] proposed a framework for multiple hypothesis testing and proved its optimality under a relaxed condition that random variables are the so-called quasi-i.i.d. in 2000.

This paper is to monitor the health of HL7 message receivers as a stochastic process. Assuming that in every time interval, say, $0, \ldots, i$, the number of received HL7s, the signal in study, is independent and normally distributed, with known different means and variances , an (on-line) algorithm for detecting mean and variance drifting faults has been derived. By using historic data learning, and adaptively additives, this algorithm can not only detect a receiverŠs status upward change; i.e., the status change from normal to abnormal, but also the downward edge. To date, the system test has been carried for several months. For all different data feeds, the fault detection for the days of non-holiday is generally satisfactory.

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Asset allocation using the Sharpe rule: how to improve an existing portfolio by adding some new assets?. **Kwok Wai Yu** (Hong Kong Polytechnic University) IC/CT4903/088

This paper discusses the applications of the Sharpe rule in portfolio measurement and management. It proposes that a portion of the portfolio value should be invested in some other assets for portfolio improvement. By applying the Sharpe rule, it can be determined that new stocks are worthy of adding to the old portfolio if they satisfy a condition, in which the average return rate of these stocks is greater than the return rate of the old portfolio multiplied by the sum of the elasticity of the VaR and 1. One attraction of our approach is diversification. A numerical example in the Hong Kong stock market is presented for illustration. Consideration is also given to the *optimal* number of new assets to be added in two specific cases (i.e., arithmetic series and geometric series regarding the sequences of expected returns and standard deviations). Some interesting simulation results show that a new portfolio with the *highest* Sharpe ratio can be obtained by adding only a few new asset.

This is work done in collaboration with Professor Xiao Qi Yang and Dr. Heung Wong.

Optimized sums in Leontjev's balance model. **Fatima Askhakova** (Karachaevo-Circassion State University, Russian Federation), Eugene Semenchin (Karachaevo-Circassion State University, Russian Federation) IC/CT4973/081

Leontjev's model of inter-industrial balance is defined as:

$$x = Ax + f, \qquad x \geq \theta, \tag{1}$$

for $x, \theta, f \in R_+^n$, where $R_+^n = \{(x_1, \ldots, x_n) \mid x_i \geq 0, i = 1, 2, \ldots, n\}$, with $A = (a_{ij})$, $i, j = 1, 2, \ldots, n$ being a non-negative matrix of dimension $n \times n$, and θ is the zero vector of dimension n. Here n denotes the number of different branches being analyzed within an economy, and x_i is the volume of output production in the i-th branch. Each a_{ij}, for $i, j = 1, 2, ..., n$, specifies the number of units of the i-th branch that is required for production of one unit of the j-th branch's output, and f is a vector of model's net production. We consider several optimized sums on a multiplicity of determinations.

(1) Maximize the gross production $\sum_{i=1}^{n} x_i$ where the x_i satisfy the Leontjev conditions. This sum measures the general gross production in the economy. It is a linear programming task to maximise it, which can be solved using known methods; e.g., the simplex method.

(2) Maximization of production volume in one or more branches. Consider criteria $x_i \to \max$ with i fixed in $1, 2, ..., n$, or $\sum_{\kappa=1}^{r} x_{i_\kappa} \to \max$, for $r \leq n$. The totality of limitations is given by the Leontjev conditions. These are analysed using balance correlations and inequalities.

(3) Maximization of production volume in several branches, taking into account their preferences. Consider maximis-

ing $\sum_{i=1}^{n} c_i x_i$, with constants satisfying $\sum_{i=1}^{n} c_i = 1$. These coefficients c_i are determined by experts and indicate the preference degree for the i-th branch over other branches.

In the case where the Leontjev model (1) is *productive* (that is, if $\operatorname{rank}(E - A) = \operatorname{rank}(E - A, f) = n$) then the maxima for all the above sums occur together, for a particular solution vector (x_i), though of course the values of the sums themselves differ. A solution of any of the above optimized sums may be assumed as a solution of the model (1) which can be used to determine any of the sums.

However if $\operatorname{rank}(E - A) = \operatorname{rank}(E - A, f) = \kappa < n$ then there can be a great number of distinct solutions for the different optimized sums, and the corresponding solution vectors (x_i) need not coincide. It is permissible to consider the optimized sums on a multiplicity of determinations (1). Solutions of (1) and solutions of the optimized sums can be different.

These results are used to analyze balance models of the economy of the Karachaevo–Circassion Republic.

IC/CTS4683/08: Finance and economics.

Organiser: Lukasz Stettner (Polish Academy of Sciences, Poland)

Long-time GOP on markets with transaction costs. **Lukasz Stettner** (Polish Academy of Sciences, Poland) IC/CT1433/081

Growth optimal portfolio (GOP) over long run time horizon is studied for markets with transaction costs. It is assumed that the asset prices (S_t) depend on economical factor process (x_t) and the pair (S_t, x_t) forms a continuous time Feller Markov process. The process (x_t) is uniformly ergodic. The dynamics of S_t is a function of x_t and an independent noise w_t. Portfolio strategy N_t is a vector which consists of numbers of assets we have at time t. For change of portfolio N_t we pay fixed plus proportional transaction costs to the volume of transaction and we assume that portfolio is self financing. Our purpose is to maximize

$$\liminf_{t\to\infty} \frac{1}{t} E\{\log V_t\},$$

where V_t is the value of the portfolio at time t. This kind of problems lead to impulsive control problems with average cost per unit time criterion. This problem in general is open. A special financial setting of the problem allows however to find solutions. In the talk various approaches to this problem will be presented. It will be shown in particular, that the problem can be approximated by discrete time problem, for which we can study suitable Bellman equation or use M. Schall approximation inequality to obtain the existence of optimal portfolio strategies. The key argument used in the talk will be based on large deviation estimates for the pair (x_t, w_t). It is also interesting that the case of proportional transaction costs (without fixed costs) in discrete time is much simpler and the optimal strategies in this case are functions of the portions π_t of the value of portfolio invested in particular assets and factor process (x_t). A few remarks concerning a partially observed case i.e. the case when economic factors (all of a part of them) are unavailable to investor will be also given. Growth optimal portfolio is important since as it will be shown it is nearly optimal for risk sensitive cost functional with risk factor sufficiently small. Part of the results presented at the talk is based on a joint contribution with dr Jan Palczewski.

Approximate formulas for zero-coupon bonds. **Gilberto Schleiniger** (University of Delaware, USA), Patrick Hagan (Brevan Howard Asset Management, UK), Fabricio Tourrucôo (Universidade Federal do Rio Grande do Sul, Brazil) IC/CT4350/081

Using perturbation methods we obtain approximate formulas for zero-coupon bonds. We present numerical simulations that partially validate the asymptotic approximation. Additionally, a calibration strategy is investigated in order to fit the model to given data on discount rates.

Stochastic rumours with an application of economics. **Selma Belen** (University of Cag, Turkey) IC/CT3082/082

In this paper, we adopt the model[1] to an investment problem. Our stochastic numerical results show that when the rumour about an investment is repeated the proportion of the population never investing approximates to 0.0049 as the population size tends to ∞.

This work is a joint work with C.E.M. Pearce.

[1] Belen, S. and Pearce, C.E.M.; Rumours with general initial conditions. ANZIAM J., 45 (2004), pp.393–400.

Numerical methods for pricing european and american options under Levy processes. **Justin Wan** (University of Waterloo, Canada) IC/CT3697/025

In this talk, we present numerical methods for solving partial integro-differential equations arising from pricing European and American options when the underlying asset is driven by a CGMY process. In the infinite activity case, the kernel of the integral term will become singular at the origin. We propose an accurate finite difference method which captures the jump component near zero by a modified diffusion. The resulting discretization yields a linear system which is dense due to the integral term. Two iterative methods are discussed for solving the discrete system effectively. Convergence analysis of the iterative methods is presented. Finally, numerical results are given to demonstrate the effectiveness of the methods.

This is a joint work with Iris Wang and Peter Forsyth.

Substitutable-inventory system with partial back-logging. **Neelamegam Anbazhagan** (Thiagarajar College of Engineering, India) IC/CT745/082

This article presents a two commodity stochastic inventory system under continuous review. The maximum storage capacity for the i-th item is fixed as S_i $(i = 1, 2)$. It is assumed that demand for the i-th commodity is of unit size and demand time points form Poisson distribution with parameter λ_i, $i = 1, 2$. The reorder level is fixed as s_i for the i-th commodity $(i = 1, 2)$ and the ordering policy is to place an order for $Q_i (= S_i - s_i)$ items for the i-th commodity (i = 1, 2) when both the inventory levels are less than or equal to their respective reorder levels. The lead time is assumed to be exponential. The two commodities are assumed to be substitutable. That is, if the inventory level of one commodity reaches zero, then any demand for this commodity will be satisfied by the item of the other commodity. If no substitute is available, then this demand is backlogged up to a certain level N_i, $(i = 1, 2)$ for the i-th commodity. Whenever the inventory level reaches N_1 or N_2, both inventory levels are pull back to its maximum level S_1 and S_2 instantaneously by canceling the previous orders. For this model, the limiting probability distribution for the joint inventory levels is computed. Various operational characteristics and expression for long run total expected cost rate are derived.

A jump telegraph model for option pricing. **Nikita Ratanov** (Universidad del Rosario, Colombia) IC/CT217/008

A new class of financial market models is developed. These models are based on generalized telegraph processes: Markov random flows with alternating velocities and jumps occurring when the velocities are switching. While such markets may admit an arbitrage opportunity, the model under consideration is arbitrage-free and complete if directions of jumps in stock prices are in a certain correspondence with their velocity and interest rate behaviour. An analog of the Black-Scholes fundamental differential equation is derived, but, in contrast with the Black-Scholes model, this equation is hyperbolic. Explicit formulas for prices of European options are obtained using perfect and quantile hedging.

08: Probability and Statistics, Posters

IC/PP4839/081: Double optimal stopping of a risk process.

Presenter: Krzysztof Szajowski (Wroclaw University of Technology, Poland)
Co-author: Anna Karpowicz (Warsaw University of Technology, Poland)

The following problem in risk theory is considered. An insurance company receives premiums and pays out claims which have occurred according to a renewal process and which have been recognized by them. The capital of the company is invested at interest rate $\alpha \in \Re^+$, the size of claims increase at rate $\beta \in \Re^+$ according to an inflation process. The immediate payment of claims decreases the company investment by rate α_1. At any moment the company may broaden or narrow down the offer, what entails the change of the parameters. This change concerns the rate of income, the intensity of renewal process and the distribution of claims. After the change the management wants to know the moment of the maximal value of the capital assets. The goal is to find two optimal stopping times: the best moment of change the parameters and the moment of maximal value of the capital assets.

The improvement to the known models is made by taking into account different scheme of claims payment and the possibility of rejection of the request by the insurance company. The proposed model takes into account different economical environments of insurance companies. It leads to essentially new risk process and the solution of optimal stopping problem is different.

IC/PP710/082: On the existence and uniqueness of a bounded mean-reverting process.

Presenter: Dharma Lesmono (Catholic University of Parahyangan, Indonesia)

We study the behaviour of a mean-reverting process described by the Stochastic Differential Equation (SDE):

$$\mathrm{d}S(t) = -\mu \frac{S(t)}{1 - S(t)^2}\,\mathrm{d}t + \sigma\,\mathrm{d}B(t)\,, \quad S(0) = S_0\,,$$

where $B(t)$ is one-dimensional Brownian motion, and μ and σ are positive constants. We prove that solution $S(t)$ remains within $(-1,1)$ whenever $|S_0| < 1$ and $\mu \geq \sigma^2$. The process behaves like the ubiquitous Ornstein–Uhlenbeck (OU) process when $S(t)$ is close to zero, but as $S(t)$ gets close to ± 1, the influence of the drift increases, thus driving the process away from the boundaries. Consequently, this SDE might be useful for modelling phenomena such as opinion polls, which have inherent maximum and minimum limits imposed.

The drift coefficient is not continuous near $S = \pm 1$. Nor does it satisfy either a Lipschitz or linear growth condition. Despite this, we will prove that there exists uniquely a solution to the SDE. We then extend this result to the case where the numerator of the drift coefficient is a polynomial in S.

Work done in collaboration with Prof. Phil Pollett (University of Queensland), Dr. Elliot Tonkes and Prof. Kevin Burrage (University of Queensland).

IC/PP4301/083: Estimations of the parameters of the smoothly-truncated Lévy distributions and their applications to EEG-sleep patterns.

Presenter: Alexandra Piryatinska (San Francisco State University, USA)

The class of Smoothly Truncated Lévy (STL_α) distributions (Koponen,1995) is an intermediate class of distributions between α-stable and normal distributions. The MM and Numerical MLE parametric estimation tools for these distributions are developed. The results are verified by simulations.

The above methods are applied to a study of the recordings of EEG sleep signals for fullterm and preterm neonates. The EEG data are not stationary. Our fist problem is to separate the time series into quasi-stationary increments. For the homogeneous increments the numerical MLE for smoothly truncated Lévy distribution is performed. The conclusion is that the STL model is appropriate for EEG-sleep patterns of fullterm babies.

[1] Koponen, I.; Analytic approach to the problem of convergence of truncated Lévy flights towards the gaussian stochastic process. Phys. Rev. E. **3**52, (1995) pp.1197–1199.
[2] Piryatinska, A.; Inference for the Lévy models and their applications in medicine and statistical physics. PhD dissertation, Case Western Reserve University, 2005.
[3] Terdic, G., Woyczynski, W. and Piryatinska, A.; Multi-scaling Properties of Time-scaled Truncated Lévy Flights, Physica Letters A, 346, (2006), pp.94–106.

IC/PP3494/085: On some new method of incorporating prior information into regression analysis and its performance in real-world applications: cross-validation analysis.

Presenter: Zbigniew Domański (Czestochowa University of Technology, Poland)
Co-author: Andrzej Grzybowski (Czestochowa University of Technology, Poland)

The presentation is devoted to the problem of incorporating prior information when estimating regression parameter. To incorporate the information together with its uncertainty into regression analysis we use estimators based upon the notion of a coefficient of uncertainty. In this presentation we focus on simulation analysis of these estimators. In our studies we use real world data, so we adopt the cross-validation technique. We compare the performance of predictors based on the considered estimators with the performance of the predictors based on the ignoring prior information least-squares estimator. The data used in presented applications are connected with steel plate properties modelling (important for steel works production management) as well as with some economic models (e.g. car or real estate market)

IC/PP3446/085: Incorporating prior information in regression estimation: on a coefficient of uncertainty based on the condition number of the matrix of observations.

Presenter: Andrzej Grzybowski (Czestochowa University of Technology, Poland)

The paper is devoted to the problem of incorporating prior information into regression model estimation. We assume the prior information about regression parameter is derived from regression analysis applied (perhaps by someone else) to some phenomenon described by the same regression equation. However, we cannot be sure that the two phenomena are described by exactly the same regression equations and we do not know how reliable the previous data and results are - the prior information is uncertain.On the base of computer simulation we construct a coefficient which allows incorporating the prior information along with its uncertainty. The coefficient is based upon the index number of the matrix of observations of the explanatory variables as well as its dimensions. Performance of estimators based upon the coefficient of uncertainty is examined through computer simulations. In the simulations the performance of the proposed estimators is compared with performance of the usual ordinary least squares estimator

IC/PP1543/015: Bootstrap estimation of the distribution of Kullback–Leibler distance in the mixed case.

Presenter: Virtudes Alba-Fernández (Universidad de Jaén, Spain)
Co-author: Dolores Jiménez-Gamero (Universidad de Sevilla, Spain)
Co-author: Joaquín Muñoz-García (Universidad de Sevilla, Spain)

In many statistical techniques, computation of a distance between two populations is often useful. For example, to test the equality of two populations one can consider some sample version of a distance between the theoretical populations as a test statistic and reject the null hypothesis for large values of the estimated distance. Let X_i, $i = 1, 2$, be two random vectors with densities f_i with respect to a σ-finite measure λ, respectively, and let $d(f_1, f_2)$ denote the symmetric version of the Kullback-Leibler distance between them.

We will assume that that each random vector X_i, $i = 1, 2$, has q continuous components and d discrete components and that it has a CG distribution, that is, the set of discrete variables define a multinomial vector with s possible states each having probability p_i, $\sum_{i=1}^{s} p_i = 1$, and conditionally on the state i, the distribution of the q continuous variables is $N(\mu_i, \Sigma_i)$.

Replacing p_i, μ_i and Σ_i, $i = 1, 2$ by its maximum likelihood estimators of we obtain the sample version of $d = d(f_1, f_2)$, say $\hat{d}$, that can be used as test statistic to test the homogeneity of both distributions. With this aim, we need to known or at least to approximate the null distribution of $\hat{d}$. As an approximation to it Bar-Hen and Daudin (J. Multivariate Anal., 53, 332–342 (1995)) have derived the asymptotic null distribution. Here we study another way to approximate it: the bootstrap. We show that the bootstrap estimates consistently the null distribution of $\hat{d}$. We also study by simulation the finite sample performance of the bootstrap distribution and compare it with the asymptotic approximation.

09: Solid Mechanics, Minisymposia

IC/MP200/009: **Configurational mechanics.**

Organiser: Ralf Müller (TU Darmstadt, Germany)
Co-organiser: Paul Steinmann (TU Kaiserslautern, Germany)
Co-organiser: Gérard Maugin (Université Pierre et Marie Curie, France)

Since the seminal works of Eshelby (1951, 1970) the general notion of configurational forces has been successfully applied in many defect situations in continuous media. The ideas of Eshelby were later picked up by many scientists to establish a theory of configurational forces, also addressed as theory of material forces. Based on different approaches the theory proves to be very valuable for the analysis of all kinds of defect situations, including point, line and surface defects or distributed inhomogeneities. The most prominent and most developed application is of course the use the configurational forces in fracture mechanics. As configurational forces are related to material inhomogeneities they have successfully been used in many material science and engineering problems with phase transitions and inelastic deformations. Also the modeling of materials with micro-structure evolution is one of the fields, in which configurational forces can provide a better understanding of processes going on within the material.

Besides these mechanically, physically, and chemically motivated situations, configurational forces are now used in computational mechanics. Especially, the combination of configurational forces and finite element methods had an impact in computational mechanics. New methods based on configurational forces are developed in numerical fracture mechanics, structural optimization and adaptivity. These methods include, for example, the so-called r- and h-adaptive methods for mesh optimization and refinement. These new developments in computational mechanics are a lively activity, which help to extend the concepts to inelastic and dynamic problems.

Reciprocity in material space. **Reinhold Kienzler** (Universität Bremen, Germany), George Herrmann (Stanford University, Tonga) IC/MT1106/009

Reciprocity relations play a prominent role in various areas of classical physics and mathematical modelling and are most useful in the solution of numerous problems. In the theory of elasticity of solids, relevant reciprocity theorems have been established during the course of the second half of the 19^{th} century by Maxwell, Helmholtz, Lamb, Betti and Rayleigh.

To recall, as an example, Maxwell's reciprocity theorem, as applied to the elastostatics of a beam, let us consider two loading states, the force F_1 applied at the position x_1 and the force F_2 applied at the position x_2. The reciprocity theorem states that the work of the force F_1 exerted at the displacement at x_1 resulting from the force F_2 is equal to the work of the force F_2 exerted at the displacement at x_2 resulting from the force F_1.

The elements of what might be called *Mechanics in Material Space*, as a counterpart of the conventional or usual *Mechanics in Physical Space* have put together by the authors in a recent monograph [1]. Material forces are interpreted as the gradient of the total energy of a body with respect to the position of a defect within the material. A material translation is understood as a change of the configuration of that body due to change in location of a defect relatively to the material in which the defect is placed.

In order to establish reciprocity in Material Space, a body is considered which contains two defects at positions x_1 and x_2, respectively. Under external load, material forces B_{10} and B_{20} can be calculated. Due to a material translation of the defect 1, say δ_1, both material forces change to B_{11} and B_{21}, whereas due to a material translation of the defect 2, say δ_2, the material forces change to B_{12} and B_{22}. By changing the order of succession of the material translation (first δ_1, second δ_2, and vice versa), a reciprocity theorem follows. Details of the derivations are given in the talk. The application of the theorem is illustrated by several examples. Especially defect-interaction problems are discussed.

[1] Kienzler, R. and Herrmann, G.; *Mechanics in Material Space with Applications to Defect and Fracture Mechanics*. Springer, Berlin, 2000.

The balance of material momentum at a shock wave propagating in a thermo-elastic material. **Manfred Braun** (Universität Duisburg-Essen, Germany) IC/MT3122/009

Any global balance law can be reduced to its local or divergence form provided the variables involved are differentiable. At a surface of discontinuity, balances are expressed by the corresponding jump conditions. By comparing the continuous and discontinuous versions of the balance laws, one can find a simple rule, how a jump condition is related to the corresponding divergence form of the underlying balance law.

The balance of material momentum can be obtained directly from the balance of physical momentum by projecting it onto the material space. This derivation, however, is valid for the continuous case only. At a surface of discontinuity, the balance of pseudomomentum is represented by a corresponding jump condition, which can be derived from the jump condition of physical momentum in a similar way as in the continuous case. If the material is assumed purely elastic, i. e., without any dependence on thermodynamic variables, the jump condition of material momentum deviates from the form that is expected on the basis of its continuous counterpart. In general, an additional source term is involved which is of third order in the strength of the shock.

The discrepancy is resolved as soon as thermodynamics is taken into account. Stress and (internal or free) energy densities now depend not only on strain but also on a thermodynamic variable (entropy or temperature), and the balance of physical momentum has to be supplemented by the energy balance. On account of these two physical balance laws, the balance of material momentum assumes the expected form, even across a singular surface. The analysis indicates that thermoelastic behavior should be taken into account to describe shock waves in elastic materials properly.

On variational sensitivity analysis and changes in the material configuration. **Daniel Materna** (Universität Dortmund, Germany), Franz-Joseph Barthold (Universität Dortmund, Germany) IC/MT1970/009

This contribution is concerned with the application of variational design sensitivity analysis in the context of structural optimization and configurational mechanics. Variational design sensitivity analysis is a branch of structural optimization, e.g. shape or topology optimization. In these disciplines we consider variations of the material configuration and we are interested in the change of the state variables and the objective functional due to these variations. These sensitivities are required in order to solve the corresponding Lagrangian equation within standard optimization algorithms.

In many engineering applications, the energy functional of the problem is used as the objective functional of the optimization problem. The first sensitivity of the energy functional with respect to changes in the design leads to the well-known weak form of the material or configurational force equilibrium, which is directly related to the energy-release rate. The second sensitivity of the energy functional provide information about

the sensitivity of the energy-release rate and yields a tangent operator in order to solve the material motion problem. Furthermore, we investigate the so-called pseudo load operator, which is derived from the sensitivity of the physical motion problem. The sensitivity of the physical as well as the sensitivity of the material motion problem depend on the structure of the pseudo load operator. Both problems are coupled by this operator and some important properties will be studied in this context. Finally, we will summarize our recent process in the theoretical as well as computational treatment by means of selected examples.

Configurational-force-based structural updates and adaptive remeshing strategies. **Dominik Zimmermann** (Universität Stuttgart, Germany), Christian Miehe (Universität Stuttgart, Germany) IC/MT3844/009

We investigate the application of configurational forces in h-adaptive strategies for elastic fracture mechanics and inelasticity. In a first step, a consistent dual physical and material thermodynamic framework of finite inelasticity is discussed. Starting from a global Clausius–Planck inequality dual equilibrium conditions are derived by a Coleman type exploitation method. From the remaining reduced global dissipation inequality the evolution equations for the internal variables are derived by the principle of maximum dissipation. Adopting these considerations to fracture mechanics, crack loading conditions as well as a normality rule for the crack propagation are obtained. In the discrete setting, the crack propagation is governed by a configurational force driven update of the underlying geometry model. The material balance equation is used to set up a h-adaptive refinement indicator. For a homogeneous body, this balance law corresponds to vanishing discrete configurational nodal forces. However, due to insufficient discretization, configurational forces occur at the interior nodes of the mesh. Their norm is used as an isotropic refinement indicator. Adopting the clear energetic interpretation of configurational forces in elasticity, where they may be related to the energetic misfit of the discretization, to problems of finite inelasticity, a relative global criterion is defined which is used for the decision on mesh refinement. Following the same reasoning, a criterion on the element level is defined which governs the local refinement procedure. The numerical treatment is carried out by coupling efficient software tools for the adaptive mesh generation, the finite element assembley and solution process, and the postprocessing step including the evaluation of the discrete configurational nodal forces. The capability of the proposed procedure is demonstrated by means of representative numerical examples.

IC/MP200/009: Configurational mechanics. #2

Organiser: Ralf Müller (TU Darmstadt, Germany)
Co-organiser: Paul Steinmann (TU Kaiserslautern, Germany)
Co-organiser: Gérard Maugin (Université Pierre et Marie Curie, France)

(For abstract, see session #1 above.)

Multiscale damage simulation. **Mario Timmel** (Universität Leipzig, Germany), Michael Kaliske (TU Dresden, Germany), Stefan Kolling (DaimlerChrysler, Germany), Ralf Müller (TU Darmstadt, Germany) IC/MT1945/009

Numerous materials often show a softening behaviour under dynamic loading. The decrease of stress, hereby, is caused by the evolution in the microscale in terms of areas where the local stiffness is reduced, e.g. due to micro-void growth. For a numerical treatment of this material behaviour, phenomenological damage approaches are used in daily engineering practice. For a better understanding of the micromechanical process of such phenomenological models, multiscale methods are becoming increasingly important. The physical quantities that are responsible for the microstructural evolution associated with the damage process are transferred to the numerical model. In this context, we use the method of configurational forces to describe the geometrical changes of damaged areas. Hereby, we present the general case of hyperelastic materials at finite strains. For the restriction of small strains, the microstructural evolution will be shown for elastoplastic materials with and without rate effects. The numerical twoscale procedure based on an explicit finite element code is presented in detail where an addition boundary value problem representing the microscale is solved in every Gaussian point. The methodology is applied to some illustrative examples.

Damage and size effects in elastic materials: a homogenization approach. **Cristian Dascalu** (Université Grenoble I, France) IC/MT2429/009

A damage model is constructed using the configurational force balance and an explict description of micro-crack evolution. We use periodic homogenization based on asymptotic developments. We show that the balance of configurational forces is able to capture size effects, which are incorporated in the resulting macroscopic damage law.

A numerical modelling based on different elementary behaviors, obtained through homogenization, allow us to take into account complex microstructural aspects like multiple microcrack orientations, unilateral contact, friction etc. We illustrate the ability of the model to reproduce known behaviors, eg. localization of damage.

Fracture mechanical investigations of rate-dependent inelastic materials at large strains. **Bastian Näser** (Universität Leipzig, Germany), Hüsnü Dal (TU Dresden, Germany), Michael Kaliske (TU Dresden, Germany) IC/MT2284/009

The material force approach is an efficient, elegant and accepted means to compute the J-integral as a fracture mechanical parameter for elastic and inelastic materials. With the formulation of a multiplicative split of the deformation gradient at hand, rate-dependent (visco-elastic) materials based on the Bergström-Boyce-Model can be investigated. For these investigations, the so-call material body forces have to be computed to separate the driving force acting on the inelastic zone around the crack tip from the driving force acting on the crack tip itself , representing the crack driving force or the J-integral, respectively. For that purpose, the complete balance for the material motion problem for rate-dependent, inelastic materials has to be known and the balance has to be fulfilled at every nodal point in a finite element discretization.

This contribution presents the formulation of the material balance and the corresponding material body forces for rate-dependent inelasticity, shows examples to prove the correctness of the formulation and implementations and gives some applications in fracture mechanics.

IC/MP327/090: Dynamics of defects in materials.

Organiser: Isaac Chenchiah (University of Bristol, UK)
Co-organiser: Thomas Blesgen (California Institute of Technology, USA)

Recent years have seen much interest in the understanding of the dynamics of defects in materials, in both the applied mathematics and engineering communities. Much progress has been made, for example, in the understanding of discrete models for defects. Further, while substantial open problems remain, sufficient progress has been made to profitably introduce the engineering community to mathematical developments. Conversely exposure to the challenges faced by the engineering community, and to the larger context in which defect motion occurs would benefit the applied mathematics community.

This minisymposium, which is addressed to both applied mathematicians and engineers, has three aims: Firstly, to facilitate interaction between researchers working on various mathematical aspects of defect motion in materials. Secondly, to review mathematical developments for researchers in the engineering community, and vice-versa. Thirdly, to stimulate interaction between applied mathematicians and engineers.

To accomplish the achievement of these goals, the minisymposium will include two review talks: one reviewing mathematical developments for a non-mathematical audience, and the other reviewing developments in the engineering community for a mathematical audience. Specific issues to be addressed in the other talks are: discrete models, passage from discrete to continuum models, multiscale aspects, and defect motion as contributing to other material phenomena.

Atomistic and continuum models of defects in solids. **Weinan E** (Princeton University, USA) IC/MT4843/090

I will give an overview of the atomistic and continuum models of defects in solids. Specifically I will discuss the dynamics of impurity diffusion, dislocation and twin boundary motion as examples of zero, one and two dimensional defects. I will discuss the atomistic mechanisms as well as continuum models for these examples.

A model of distributed faulting in confined brittle materials. **Anna Pandolfi** (Politecnico di Milano, Italy), Sergio Conti (Universität Duisburg-Essen, Germany), Michael Ortiz (California Institute of Technology, USA) IC/MT4833/090

We present a model of distributed damage in brittle materials undergoing triaxial compression. We aim to compute the effective or macroscopic behavior of the material from its elastic and fracture properties; and to predict the microstructures underlying the microscopic behavior. Additionally, we present the numerical implementation of the damage model within a concurrent multiscale framework, and the validation of the model against the experimental data of pertaining to compressive damage in confined ceramics.

Processes of distributed damage in brittle materials have been modelled by a variety of means. Local models of distributed damage have been in some cases misapplied to processes of fracture in brittle solids under tension, where fracture mechanics is expected to govern the behavior of the solid. One of the aims of the present paper is to elucidate the conditions under which damage occurs in a distributed fashion, and therefore can be described by a damage model. We show that distributed damage, as opposed to fracture, is a compressive phenomenon and only occurs when sufficient confinement is present.

The approach followed in the present paper is based on methods of the calculus of variations. We suppose that the displacement field jumps discontinuously across a singular set of co-dimension 1, and that the energy is composed of two terms: the elastic strain energy obtained by volume integration outside the singular set; and the cohesive fracture energy obtained by surface integration over the singular set. However, in contrast to recent work on free-discontinuity problems in fracture mechanics, that has emphasized tensile conditions leading to the formation of isolated dominant cracks, here we envision conditions of triaxial compression resulting in a distributed singular set. We specifically consider singular sets that are composed of recursive or nested faults, and show that these microstructures or damage patterns suffice to fully relax the energy.

A recursive fault pattern may be constructed by introducing into the solid a family of parallel planar cohesive cracks, or faults, and subsequently applying that construction recursively to the intervening matrix between the faults. The state of stress within each level of faulting is uniform, and therefore in equilibrium, although the different levels of faulting are only approximately compatible. Recursive faulting can be implemented simply by means of a recursive call, and the entire microstructure needs not be considered at any time during the construction. The approximate compatibility between levels of faulting has the effect of building additional misfit elastic energy into the microstructure. We estimate this misfit elastic energy simply by modelling the approximate interfaces as rows of dislocation dipoles. This simple estimate permits the calculation of the separation between the faults, and provides a natural termination criterion for the recursive faulting algorithm.

Homogeneous nucleation of dislocations. **Ana Carpio** (Universidad Complutense de Madrid, Spain) IC/MT4853/090

We present a mathematical theory of nucleation of dislocations is crystals. The dynamics of crystal atoms is described by a discrete elasticity model with a periodic dependence on discrete strain which changes with the type of bond. In a perfect 2D cubic lattice, dislocations are nucleated when a large enough shear stress is applied and then move towards the boundary. The resulting pattern depends on the magnitude of the load, the size of the crystal and the periodic nonlinearity. Nucleation corresponds to a bifurcation in the branch of solutions describing sheared lattices as the shear grows. We are able to predict the critical stress for nucleation and the location of nucleation sites.

Relaxation and microstructure formation in single-crystal plasticity. **Sergio Conti** (Universität Duisburg-Essen, Germany) IC/MT4845/090

This contribution deals with single-crystal plasticity with large latent hardening, which signifies that deformations which are single slip at each material point are favored. The resulting nonconvexity of the incremental variational problem induces the formation of fine-scale structures. In a geometrically nonlinear framework, and with rigid elasticity, an explicit relaxation is obtained for the case that a single slip system is active (in the two directions), both without self-hardening and with linear self-hardening. Our construction shows that laminates are formed, and that plastic deformation is present only in one of the two phases. We then extend the result to the non-rigid case, still with only one active slip system. This is done by combining a partial analytical relaxation with a numerical relaxation algorithm. The latter contains both a local optimization of the laminate and a check for optimality, based on the construction of a polyconvex lower bound. As a second example, the full set of fcc slip systems is considered, within linearized kinematics. We show that, by developing microstructures in the form of sequential laminates of finite depth, crystals can beat the latent hardening. The relaxed constitutive behavior is indistinguishable from multislip ideal plasticity. We find, however, that relaxation requires the introduction of slip lines in the microstructure, i.e., lines of concentrated slip and discontinuous displacement.

IC/MP3479/092: Higher-order asymptotic homogenisation and wave scattering in periodic composite structures.

Organiser: Igor Andrianov (RWTH Aachen, Germany)

Many studies in the theory of composite materials are based on the exploitation of the classical continuum model assuming that the original heterogeneous medium can be substituted by a homogeneous one with certain homogenized (so called effective) mechanical properties. However, this idealized assumption can not be applicable to a number of practical problems. In real composites the micro structural scale effects may result in specific non-local phenomena which can not be predicted in the frame of the homogenized medium theory.

Scale effects can be systematically analysed by means of the higher-order asymptotic homogenization method (AHM). In static problems the heterogeneity of the medium results in the induction of an infinite series of displacement fields with successively lower amplitudes. On macro level, instead of homogenized equilibrium equations of continuum mechanics we obtain new equilibrium equations that involve higher order spatial derivatives and thus represent the influence of the micro structural heterogeneity on the macroscopic material's behaviour.

In dynamic problems the physical role of the scale effects is even more significant. When the wavelength of a travelling signal becomes comparable to the characteristic size of heterogeneities, successive reflections and refractions of the waves at the components' interfaces lead to the formation of a complicated sequence of so called pass and stop frequency bands. In this case the composite plays a role of a discrete frequency filter. Application of the AHM provides a long-wave approach valid in the low frequency range. Solution for the high frequencies can be obtained on the basis of the Floquet–Bloch theorem by one of the following approaches: the plane-wave expansions method, the Rayleigh multipole-expansions method, and the Korringa–Kohn–Rostoker method (also known as the multiple scattering method).

The aim of the minisymposium is the presentation and the comparative analysis of the modern approaches for the higher-order simulation of periodic composite structures taking into account the scale effects and the wave scattering phenomena.

Study of wave dispersion in periodic composites by higher-order asymptotic homogenization method. **Vladyslav Danishevskyy** (Prydniprovska State Academy, Ukraine), Igor Andrianov (RWTH Aachen, Germany), Vladimir Bolshakov (Prydniprovska State Academy, Ukraine), Dieter Weichert (RWTH Aachen, Germany) IC/MT3882/092

In the present work an application of the higher-order asymptotic homogenization method (AHM) to the study of wave dispersion in periodic composite structures is considered. It should be noted that the most significant and practically important phenomena caused by the heterogeneity of the composite media arise in dynamic problems. When the wavelength of a travelling signal becomes comparable to the size of heterogeneities, successive reflections and refractions of the waves at the components' interfaces lead to the formation of a complicated sequence of so called pass and stop frequency bands. In this case the composite plays a role of a discrete frequency filter.

As illustrative examples we study propagation of harmonic elastic waves in a layered composite (one-dimensional problem allowing the exact analytical solution) and in a fibre-reinforced composite with a square lattice of cylindrical inclusions (two-dimensional problem). The asymptotic homogenization schemes are developed and the higher-order macroscopic wave equations are derived. Analysis of the obtained solutions shows that the AHM provides a long-wave approach valid in the low frequency range. Solutions for the high frequencies are obtained on the basis of the Floquet-Bloch theorem by expanding spatially varying material properties in Fourier series and representing unknown displacement fields by infinite plane-wave (PW) expansions. However, this approach may run into convergence problems with the increase in contrast between the components properties. Eventually, we can conclude that the higher-order AHM and the PW expansions method can be treated as complementary to each other. The dispersion curves relating the wave numbers and frequencies are obtained; the pass and stop frequency bands are identified; the attenuation factors within the stop bands are evaluated.

Long-wave scattering by a periodic distribution of oscillators on the free surface. **Claude Boutin** (ENTPE, France) IC/MT3922/092

This article is devoted to wave propagation in presence of a periodic distribution of oscillators (3D spring-damped masses) on the surface of an elastic medium. The case of an elastic half-space loaded by quasi-periodic surface forces is studied first. The equivalent boundary conditions at the macro-scale are derived at the first and second order, by assuming the existence of a boundary layer and using a two-dimensional homogenisation method. When the force distribution results from attached oscillators, it is shown that boundary conditions can be expressed in terms of equivalent surface impedance at the first order, with local and non local correctors at the second order. These results are used to study wave refraction by an oscillator layer. The main phenomena - atypical redistribution of mode and mode conversion, frequency range of efficiency, characteristic time of response - are identified. The first correctors are determined analytically for plane waves of oblique incidence. Finally the validity range of the modelling is discussed.

Wave propagation and diffraction in discrete structures: effect of anisotropy and internal resonance. **Claude Boutin** (ENTPE, France), Celine Chesnais (Ecole Nationale des Travaux Publics de l'Etat - CN, France), Hans Stephane (ecole Nationale des Travaux Publics de l'Etat - CN, France) IC/MT4072/092

This paper is devoted to the study of wave propagation within discrete periodic bi-dimensional structures. The problem is tackled by considering a class of structures made of repeated un-braced frames. The behaviour of these frame structures is determined by the distribution of shear force and inner bending in the elements according to their mechanical and geometrical characteristics. Moreover, since resisting elements are only present in two directions, the global system is highly anisotropic.

Assuming the frame size is small compared to the wavelength, the macroscopic equivalent descriptions are obtained by the homogenization method of periodic discrete media. Depending on the considered frame structure and on the order of magnitude of the frequency (relatively to the scale ratio) several families of waves are proven to be possible. Increasing the order of the frequency one obtains:

- pure shear waves propagating in the direction of the frame, while in other directions the regime remains quasi-static;
- modes of shear-compression waves. At this level of frequency the elements reach their resonance (in bending). This internal resonance leads to a frequency depending apparent mass of the system that in turn, induces a dispersion of waves. Note that the quasi-Shear mode propagates except in the directions of the frame (in these directions the diffraction regime is already reached), and the quasi-compression mode reduces to pure compression waves in the directions of the frame.
- full-diffraction range where no propagation modes can exist.

These theoretical results show that the high anisotropy induces very separated diffraction frequencies according to the considered modes. Therefore propagation and diffraction may occur conjointly at the same frequency. To conclude analogies with micromorphic media are discussed.

Continuous models of discrete media valid for the high-frequency domain. **Igor Andrianov** (RWTH Aachen, Germany) IC/MT4151/092

Microstructural effects play a significant role in the mechanical behaviour of heterogeneous materials and are essential in problems of damage mechanics, molecular dynamics, theory of plasticity, mechanics of composites, nanomechanics.

These effects can be taken into account using either discrete or continuous models. Let us focus on the continuum description of the dynamic behaviour of microstructural materials. Each component can be modelled separately by means of the classical continuum, and then the microstructure is considered as a heterogeneous classical continuum. On the other hand, a homogeneous continuum can be used and the influence of the microstructure can be taken into account by averaging. Here three strategies exist: the phenomenological approach (additional terms are added to the energy functional or to the constitutive relation; the structure and character of these terms are postulated), the statistical approach (starting from a heterogeneous classical continuum average values of the state variables are computed to produce enhanced field equations), and the homogenization approach (based on G-limit technique). The applicability of all the above mentioned models in dynamics is restricted to limited ranges of frequencies. At high frequencies, these models either become unstable or presume an infinite speed of the energy propagation. From a physical standpoint, the inapplicability of homogeneous continuum models at high frequencies is fully justified, since the heterogeneity and anisotropy of microstructural materials cannot be ignored as the wavelength size approaches the span of the microstructural irregularity.

We propose a new approach to obtain explicit relations between micrtostructural properties and microstructural parameters. It is based on the asymptotic construction of two limiting cases and further using of two-point Padé approximants.

IC/MP697/092: Geometric and stochastic aspects of the mechanics of complex bodies.

Organiser: Paolo Maria Mariano (Università degli Studi di Firenze, Italy)
Co-organiser: Thomas Pence (Michigan State University, USA)
Co-organiser: Eric Vanden-Eijnden (Courant Institute, NYU, USA)

Stringent industrial requirements of sophisticated performances and of circumstantial control for micro-devices or nanotechnology manufactures (and other types of machinery at multiple scales) can be often satisfied only by resort to or allowance for complex materials. The adjective *complex* beckons to the fact that the substructure influences the gross mechanical behaviour in a prominent way by means of interactions due to substructural changes, interactions that have to be represented directly generating non-trivial geometrical questions. Moreover, geometry plays a crucial role above all to underline the invariant (or better covariant) structures of the models one manages. There is a crucial interplay between geometry and analysis when one looks for the possibility of finding solutions or at least relevant existence theorem, as it occurs in evaluating the existence of ground states of elastic complex bodies. The description of the mechanical behaviour of complex bodies proposes a wide class of challenging problems of mathematical, physical and computational nature from macroscopic-to-nano-world. However, substructures are not necessarily micro or nano; for example in turbulence of polymeric fluids the formation at mesoscopic level of coherent structures due to the interplay between macroscopic motion and microscopic self-organization of polymeric chains influences drastically the whole scenario of the macroscopic motion. This is just an example, of course. Stochastic effects occur in prominent cases as the segregation of phases, turbulence of complex fluids and the interaction between phonon and phason modes in quasicrystals. These effects may also be rare events of crisis. Finally, computations require non standard methods involving approximations over manifolds. In working about complex bodies one becomes aware that often points of departure that seem of disparate nature manifest at the end unexpected connections and common foundations.

The basic aim of the proposed minisymposium is to show different aspects of the mechanics of complex bodies from theory to computations and the subtle connections between them, paying above all attentions on geometrical and stochastic questions arising from physical modelling and on the related computational problems.

A quest for an extended *continuum mechanics.* **Gianfranco Capriz** (Università di Pisa, Italy) IC/MT3190/092

Earlier reflections on balance equations possibly appropriate for hyperfluids or pseudofluids (reflections broached originally so as to dispose of lack of strict objectivity in standard thermal quantities) are instanced again with a different slant. It is alleged that partially chaotic motions can be efficiently branded by assigning pertinent averages, moments and variances and these gauges can be all (not only the first two) considered mechanical; hence the qualifier 'extended'. A few immediate consequences of the approach are derived, open problems are listed, connections or dissensions with widely acknowledged notions are discussed.

Shearing deformations for a class of elastic materials with an internal balance based on a decomposition of the deformation gradient . **Thomas Pence** (Michigan State University, USA), Hasan Demirkoparan (Carnegie Mellon - Qatar) IC/MT2440/092

In order to model certain substructural reconfigurations in solids we consider a standard multiplicative decomposition of the deformation gradient and consider constitutive laws based on separate energy minimization of the decomposition factors. It is found that even very simple constitutive laws formulated on this basis give rise to interesting possibilities for localized deformation. This is demonstrated in boundary value problems involving shearing wherein certain applied traction thresholds, or applied shear thresholds, give rise to energy minimizers involving discontinuity of deformation in an appropriate limiting sense.

Small-scale anisotropy in shear turbulence. **Massimo Casciola** (Università degli Studi di Roma "La Sapienza", Italy) IC/MT2461/092

According to Kolmogorov, isotropy is recovered in the large Reynolds number limit as the scale is reduced and, in the so-called inertial range, universal features (namely the scaling exponents of structure functions) emerge clearly. However this picture is violated in a number of cases, typically in the high shear region of wall bounded flows. The common opinion ascribes this effect to the contamination of the inertial range by the larger anisotropic scales; i.e., the residual anisotropy is

assumed as a weak perturbation of an otherwise isotropic dynamics. This kind of reasoning fails when the anisotropic effects are strong as in the production range of shear dominated flows. This regime is analyzed here by means of both numerical and experimental data for a homogeneous shear flow. A well defined scaling behavior is found to exist, with exponents which differ substantially from those of classical isotropic turbulence. A systematic use of the $\mathrm{SO}(3)$ decomposition on the correlation tensors of velocity fluctuations enables to extract the different anisotropic contributions. They vanish at small scale at a relatively fast rate under weak shear. Under strong shear instead they keep a significant amplitude up to viscous scales, thus leaving a signature on the gradients.

Finally, the general validity of these results is discussed in the context of applications, where more appropriate closure models would be advisable. In fact, as we will show, commonly we find conditions under which statistical isotropy is never recovered and where the anisotropy induced by large scale shear contaminates the entire range of scales up to velocity gradients.

Asymptotic analysis and relaxation of Mumford–Shah type energies with obstacles. **Matteo Focardi** (Università di Firenze, Italy) IC/MT2512/092

Homogenization of particle-reinforced composites and porous bodies may involve minimum problems for Mumford–Shah type functionals with obstacle conditions. For bodies with a periodic distribution of holes, one may be interested in analizing the behaviour of the (say) elastic energy as the diameter of the holes tends to 0. By selecting the Dirichlet energy as a prototype, one analizes the asymptotics as ε tends to 0 of mimimum problems of the type

$$\inf\left\{\int_\Omega |\nabla u(x)|^p \mathrm{d}x + \mathcal{H}^{n-1}(S_u) + \text{ lower order terms} : u \in SBV(\Omega),\ u = 0 \text{ on } \mathbf{B}_\varepsilon \text{ and } \Omega,\right\}$$

where $\Omega \subset \mathbb{R}^n$ is a given regular bounded open set, ∇u and S_u are, respectively, the (approximate) gradient and the set of (approximate) discontinuities of u, and $\mathbf{B}_\varepsilon = \Omega \cap \cup_{\underline{i}\in\mathbb{Z}^n} B_{r_\varepsilon}(\underline{i}\varepsilon)$, with $B_{r_\varepsilon}(\underline{i}\varepsilon)$ the ball centered in $\underline{i}\varepsilon$ of radius $r_\varepsilon > 0$.

The restriction to the Sobolev space $W^{1,p}$, $p > 1$, is classical and has been analyzed in many works after the pioneering results by Marchenko and Khruslov [5], Rauch and Taylor[6,7] and Cioranescu and Murat[2].

The limit energy to be minimized contains an extra term which is a finite penalization keeping track of the local capacity density of the homogenizing obstacles (with the appropriate notion of capacity related to the Dirichlet type energy under consideration). In order to deal with this *relaxation phenomenon*, De Giorgi, Dal Maso and Longo[4] proposed an approach via Γ-convergence arguments for the associated Dirichlet energies[1,3].

Along this line, and taking into account the general case of unilateral constraints, we consider the functionals

$$F_\varepsilon(u) = \int_\Omega |\nabla u|^p \mathrm{d}x + \mathcal{H}^{n-1}(S_u) \quad u \in SBV(\Omega),\ u = 0\ \mathcal{L}^n \text{ a.e. on } \mathbf{B}_\varepsilon,$$

$+\infty$ otherwise in $L^1(\Omega)$, and show that (F_ε) Γ-converges in the L^1 topology to

$$F(u) = \int_\Omega |\nabla u|^p \mathrm{d}x + \mathcal{H}^{n-1}(S_u) + n\omega_n \beta^{n-1} \mathcal{L}^n(\{x \in \Omega : u(x) \neq 0\}),$$

where the coefficient β is finite and different from 0 if and only if $r_\varepsilon \sim \varepsilon^{\frac{n}{n-1}}$.

The term $n\omega_n$ is a capacity related to the *functional capacity of degree 1* of the reference hole $B_1(\underline{0})$. Here, we prove the Γ-convergence result for a generic reference perforation set E by replacing in the limit energy $n\omega_n$ with the 1-capacity of a suitable $\mathcal{L}^n$ representant of E. Moreover, we give an equivalent formulation of the obstacle problem for reference perforations with Lebesgue measure zero[8]. Eventually, we characterize the lower semicontinuous envelope of Mumford–Shah type energies with pure obstacles and show that it can be written by means of an $(n-1)$-dimensional variational measure introduced by De Giorgi in the study of minimal surfaces with obstacles [9].

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IC/MP697/092: Geometric and stochastic aspects of the mechanics of complex bodies. #2

Organiser: Paolo Maria Mariano (Università degli Studi di Firenze, Italy)
Co-organiser: Thomas Pence (Michigan State University, USA)
Co-organiser: Eric Vanden-Eijnden (Courant Institute, NYU, USA)

(For abstract, see session #1 above.)

Geometric models of internal structure and their group analysis. **Jan Slawianowski** (Polish Academy of Sciences, Poland) IC/MT3883/092

Suggested is a class of geometric models of bodies which are complex on the micro- and nano-level. Degrees of freedom of the internal structure of material elements are modelled with the use of homogeneous spaces of some transformation groups suggested by the very geometry of the physical space, like the real affine or unitary group and their subgroups. On the basis of the powerful methods based on group theory performed is a qualitative analysis and also analytical computations concerning the micro- and nano-dynamics. Quantization aspects are discussed because this realm of phenomena is characterized by the convolution and overlaping of the classical and quantum levels of description.

Boundary roughness effects in nematic liquid crystals. **Paolo Biscari** (Politecnico di Milano, Italy) IC/MT3617/092

Nematic liquid crystals possess three different phases: isotropic, uniaxial, and biaxial. The ground state of most nematics is either isotropic or uniaxial, depending on the external temperature. Nevertheless, biaxial domains have been frequently identified, especially close to curved surfaces. In the first part of the talk we show how the surface curvature tensor may be a source of biaxiality[1]. We then show how the boundary conditions weaken if the boundary roughness increases, and relate the microscopic roughness parameters to an effective anchoring potential, that replaces the (strong) boundary conditions[2].

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Fluid dynamics of an open quantum system in the high-field regime. **Chiara Manzini** (Università degli Studi di Firenze, Italy), Giovanni Frosali (Università degli Studi di Firenze, Italy) IC/MT3705/092

Electronic devices operating in high-field regimes have become subject of interest for semiconductor modelists. Simulations of these devices were based on fluiddynamical models with parameters adapted to experimental values. More recently, novel models with field-dependent parameters have been proposed. The derivation of *quantum* macroscopic models from kinetic ones as in gasdynamic theory is delicate both from the analytical and the physical point of view. The conservative dynamics of the isolated quantum system has to be broken, by taking into account dissipative interactions with the environment; however, when considering the weak coupling of the system with the environment, a Markovian dynamics can still be adopted. A discussion of physically-consistent quantum kinetic models shall be proposed. Then, we shall consider the high-field Wigner-BGK equation and derive quantum drift-diffusion and quantum hydrodynamic models, containing *explicit* field-dependent terms.

Einstein relation on fractal objects. **Uta Renata Freiberg** (Australian National University) IC/MT4055/092

Many physical phenomena proceed in or on irregular objects which are often modeled by fractal sets. Using the model case of the Sierpinski gasket, the notions of Hausdorff, spectral and walk dimension are introduced. These "characteristic" numbers of the fractal are the "ingredients" of the Einstein relation, expressing the interaction of geometric, analytic and stochastic aspects of a set.

em Keywords*: fractals, self-similarity, Hausdorff dimension, Dirichlet form, Laplacian, spectral dimension, (strong) Markovian process, walk dimension, Einstein relation*

IC/MP56/092: Modeling, analysis and simulation of crystal defects: dislocation and surface step dynamics across the scales.

Organiser: Yang Xiang (Hong Kong University of Science and Technology)
Co-organiser: Dionisios Margetis (Univ. Maryland at College Park, USA)

Crystalline materials are used extensively in the design and fabrication of novel devices. The modeling of such materials, especially their defects, is an area of active research with numerous analytical and computational challenges. This minisymposium focuses on recent advances in the modeling, analysis and simulation of line defects inside crystals (dislocations) and on crystal surfaces (steps). These defects are of atomic size, but they influence the properties of crystals and the corresponding devices at mesoscopic and macroscopic length and time scales. This influence can be due to long-range elastic effects, or to boundary conditions of atomistic (hence, discrete) origin at macroscopic free boundaries. From the viewpoint of physical phenomena, the collective behavior of dislocations determines the plastic deformation of solids; and the motion of steps determines the surface morphology and the lifetimes of nanostructures. From the standpoint of modeling, the atomistic models provide detailed information for the mechanics near the defects; and, on the other hand, continuum models enable predictions at sufficiently large length scales. Hybrid-like theories across scales are also being developed, which, for example, couple simpler models through different length scales, or incorporate useful atomistic detail into continuum models. The invited speakers of this minisymposium will address different aspects of these physical phenomena and modeling approaches, including novel mathematical problems that emerge from them.

Multiscale modeling and simulation for thin film growth. **Russel Caflisch** (University of California, Los Angeles, USA) IC/MT2074/092

This talk presents an application of multiscale modeling and simulation to epitaxial growth of thin films. We describe growth models at three different scales: Monte Carlo atomistic models, island dynamics models and continuum models. The atomistic models include random deposition and hopping of atoms on a lattice. Island dynamics models are coarse-grained in the lateral directions, but are atomistically discrete in the growth direction. They describe step edges and island boundaries as continuous curves. Continuum models are coarse-grained in all directions and describe the epitaxial surface through a continuous height function. Connections between these models are a principal goal of mathematical materials science.

Nonlinear instabilities and shape evolution for single-layer islands. **Joachim Krug** (Universität zu Köln, Germany) IC/MT2006/092

The nonequilibrium evolution of two-dimensional nanoscale structures is a central theme in current surface science. The key theoretical challenge is to bridge the length and time scales between individual atomic processes and the mesoscopic step morphologies that they produce. A highly successful approach to this problem treats the crystal steps as continuous entities, whose dynamics is governed by the interplay between the adatom population on the terraces and the processes at the steps. Depending on whether mass transport occurs predominantly along the step or across the terraces, this results in a local or nonlocal boundary evolution problem. In this talk I report recent progress in the step-dynamical modeling of electro-migration-driven island motion. In the first part the focus is on the local regime, where the problem becomes equivalent to the driven motion of a dislocation loop. The incorporation of crystal anisotropy in the step atom mobility is shown to lead to complex shape evolution scenarios, which include spontaneous symmetry breaking and oscillatory as well as chaotic time dependencies[1]. The predicted behaviors were recently verified in kinetic Monte Carlo simulations of a realistic model for the Cu(100) surface, and quantitative agreement was achieved using suitably parametrized expressions for the

step stiffness and the step atom mobility[2]. In the second part of the talk I consider the nonlocal problem of driven migration of vacancy islands with interior terrace diffusion. In the limit of a strong attachment asymmetry (Ehrlich–Schwoebel effect), a circular island moves at constant speed and remains linearly stable, but a nonlinear instability resulting in the pinch-off of a small island occurs for large driving[3].

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Microscopic modelling of the dynamics of crystal surfaces in presence of a macroscopic electric field, and its consequences on spontaneous pattern formation on the nano-scale. **Olivier Pierre-Louis** (Université Joseph Fourier Grenoble, France) IC/MT2151/092

In presence of an electric current in the bulk of a crystal, surface atoms experience a drift, which is called electro-migration. This drift induces a macroscopic mass flux along the surface. Such a mass flux depends on the local geometry, and may redistribute the mass on the surface, thereby creating patterns on the micro or nanometer scale. The understanding of these morphological changes of the surface requires to link the dynamics at different lengthscales: starting from the drift experienced by a single mobile atom at the surface, how can one determine the macroscopic evolution? We will see how the introduction of a intermediate (meso-scopic) lengthscale allows one to handle these changes of scale. The relevant structure at an intermediate lengthscale is the atomic step on the crystal surface. We will first focus on the derivation of the equations of motion of these atomic steps from a microscopic model called a phase field model. We will also discuss how the dynamics of these steps may account for the macroscopic dynamics of the surface.

Crystal surface evolution: from discrete schemes to continuum laws. **Dionisios Margetis** (Univ. Maryland at College Park, USA) IC/MT1027/092

In traditional settings such as fluids and classical elasticity the starting point ("truth") often takes the form of continuum equations for macroscopic variables of interest. But in the modeling of crystalline materials this perspective needs to be changed: The truth is atomistic, or takes the form of discrete schemes, by which evolution laws must be derived at the macroscale. On the basis of this approach predictions can be made for the design, fabrication, and properties of novel solid-state devices. In this talk I focus on recent progress in elucidating the relation of discrete schemes to continuum laws in crystal surface evolution. The governing, discrete equations represent the motion of interacting line defects, "steps" with atomic height. In the appropriate continuum limit nonlinear PDE's are derived for the surface motion. Remarkably, isotropic physical effects at the nanoscale give rise to anisotropies at the macroscale. The PDE's can properly describe the onset of instabilities, particularly "step bunching", by which a continuum description may break down. I will discuss the cases with near- and far-from-equilibrium step kinetics, and progress as well as challenges in the formulation of a continuum theory.

IC/MP56/092: Modeling, analysis and simulation of crystal defects: dislocation and surface step dynamics across the scales. #2

Organiser: Yang Xiang (Hong Kong University of Science and Technology)
Co-organiser: Dionisios Margetis (Univ. Maryland at College Park, USA)

(For abstract, see session #1 above.)

Dislocation dynamics simulations in thin films using the level-set method. **Yang Xiang** (Hong Kong University of Science and Technology) IC/MT1452/092

The control of the density and location of dislocations (line defects) in heteroepitaxial thin film is very important in designing semiconductor-based electronic devices. We have developed a level set method based, three dimensional dislocation dynamics simulation method to describe the motion of dislocations in thin films. The dislocation location is given by the intersection of the zero level sets of a pair of level set functions. This representation does not require discretization and tracking of the dislocation, and handles topological changes automatically. The simulation method incorporates the elastic interactions of the dislocations and the stress fields throughout the film and substrate. Using the above approach, various dislocation motion and interactions within a heteroepitaxial thin film are simulated and analyzed.

Large-scale dislocation dynamics simulations: applications to strength in bulk and finite size systems. **Meijie Tang** (Lawrence Livermore National Laboratory, USA) IC/MT2540/092

This talk will present a front-tracking dislocation dynamics method. The dislocation dynamics method is a numerical tool to quantitatively describe plasticity and strength in crystalline materials. It tracks the collective motion of dislocation line defects and their interactions. It evolves the microstructure formed by the dislocation lines and predicts the yield strength and strain hardening properties. Applications have been made using the LLNL large scale parallel dislocation simulator (ParaDiS) for both bulk and finite sized metallic systems. In these applications, the dislocation dynamics simulations are found to be powerful tools to discover new microstructure [Nature, 440, p1174 (2006)], understand strength in bulk systems, and to explore mechanisms responsible for 'the smaller, the stronger' observation in micro- and submicro- systems in recent experiments.

From electrons to finite elements: a concurrent multiscale approach for metals. **Gang Lu** (CSU Northridge, USA) IC/MT2025/092

We have recently developed a powerful multiscale modeling approach that concurrently couples quantum mechanical calculations for electrons, to empirical atomistic calculations for classical atoms, and to continuum mechanical calculations for finite elements, in a unified description [1]. In specific, the electronic calculations are performed with the plane-wave pseudopotential method based on the density-functional theory (DFT), the classical atomistic simulations with the embedded-atom method (EAM), and the continuum calculations with the Cauchy-Born rule in the local Quasicontinuum (QC) formulation [2]. The multiscale method is implemented in the context of the QC framework with the additional capability to include DFT

calculations for a selection of non-local QC atoms. A novel coupling scheme has been developed to combine the DFT and EAM calculations [3] in a seamless fashion to deal with non-local QC atoms, whereas the local QC atoms are treated in the usual way by the informed finite element calculations. We apply this method to study an edge dislocation in aluminum in the absence and presence of hydrogen impurities at the core. We compare our results to those from the original QC and other atomistic methods. It is clear that our method can provide more accurate descriptions for the defect core properties thanks to the DFT calculations, and yet it can treat much larger systems than standard atomistic and DFT methods thanks to the local QC formulation. If time permits, I will also talk about our recent studies on ductile fracture of Al using the same method.

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Generalized Peierls–Nabarro models for curved dislocations. **Pingbing Ming** (Chinese Academy of Sciences), Yang Xiang (Hong Kong University of Science and Technology) IC/MT2058/092

Peierls–Nabarro model is a way of incorporating crucial atomistic features into a continuum framework. Originally it was proposed as a qualitative model for dislocations in solids in order to overcome certain difficulties associated with the continuum theory of dislocations. Subsequent work has greatly improved the accuracy of the model, making it a useful quantitative tool for dislocation structure and dynamics. In this talk, we present a systematic approach for developing accurate Peierls-Nabarro models for general curved dislocations and general crystal structures, in which the dislocation core structure is obtained by the minimization of the total energy including the elastic energy and the energy due to the nonlinear interaction across the slip plane (the misfit energy). We present efficient numerical methods for treating the anisotropic elastic contributions. We also discuss two different ways of developing models for the misfit energy density, the generalized stacking fault energy: one based on symmetry consideration and the other based on direct summation using atomistic potentials. Examples are given for the core structures of straight dislocations and dislocation loops in Al and Cu. I will also talk about the theoretic aspects of this model, in particular, the local and global existence results.

This is a joint work with Yang Xiang (Hong Kong University of Science and Technology), He Wei (Peking University) and Weinan E (PACM, Princeton University).

IC/MP191/093: Dense granular systems: from theory to applications.

Organiser: Lou Kondic (New Jersey Institute of Technology, USA)
Co-organiser: Corey O'Herrn (Yale University, USA)

Dense granular materials appear in a host of applications from the handling of industrial materials to pharmaceutical powders and are relevant to a number of natural phenomena. While significant progress has been reached in understanding dilute systems via kinetic theory and its extensions, progress in the field of dense, slowly sheared systems has been much slower. The issues such as jamming, strong fluctuations of relevant flow properties, history dependence, to name just a few, require development of new research methods. These methods, which vary from discrete modeling via molecular dynamics simulations, extensions of equilibrium statistical mechanics, to development of mesoscale models, reflect multiscale issues which are intrinsic to dense granular systems. The talks in this minisymposium give a wide overview of the current state of the art in this important field, and will cover the topics which will vary from fundamental mathematical issues to applications of granular materials in industrial settings.

Mechanisms for energy dissipation in dense cohesionless granular assemblies: implications for shear banding interpreted as a bifurcation phenomenon . **Antoinette Tordesillas** (University of Melbourne, Australia) IC/MT2819/093

The formation and evolution in two-dimensions of the so-called *persistent shear band* in densely packed assemblies of cohesionless particles are examined using two methodologies: bifurcation analysis within the framework of micromechanical continuum theory and discrete element method (DEM). The former is based on a general micropolar or Cosserat constitutive law, from which several conclusions can be made about the post-bifurcation evolution of the shear band. While many of these conclusions do not depend on the details of the constitutive law, a key advantage of micropolar theory is its link to micromechanically based constitutive laws. It is through micromechanics that a direct link can be made between the mathematical continuum model and observations of the discrete material using particle-based numerical (DEM) and/or experimental techniques.

The motivation for the two-dimensional bifurcation analysis stems from our recent DEM studies which demonstrate that the alternating formation and collapse (via buckling) of load-bearing particle columns or force chains characterize the steady-state (Ṣpersistent T̆) evolution of shear bands, and constitutes the governing mechanism for energy dissipation. Recent experimental findings [1] support these results and further suggest that these mechanisms may be responsible for the observed periodic pattern in the displacements along the shear band axis. The bifurcation analysis shows that a displacement field which is periodic along the shear band axis and displays odd-symmetry across the shear band, leads to a closed form solution for the shear band width. We also show that shear banding is possible in the absence of Cosserat effects Ű in contrast with the one-dimensional bifurcation theory which predicts that shear bands cannot form in the absence of rotational degrees of freedom.

[1] Rechenmacher A (2006), Journal of the Mechanics and Physics of Solids, 54 pp 22Ű45.

Microstructural studies of dense granular media and their importance to the pharmaceutical industry. **Meenakshi Dutt** (University of Cambridge, UK), James Elliott (University of Cambridge, UK) IC/MT4888/093

Granular materials are agglomerates of particles (10 microns to 10 meters) which interact with one another via dissipative contacts. We will be presenting numerical investigations (using Discrete Element Method (DEM) techniques) of dense granular media generated by gravity settling and constant strain uni-axial compression. The particle size distribution chosen in our study is motivated by X-ray microtomography scans of pharmaceutical excipient compacts (X. Fu *et al.*, Powder Technology 2006). We will discuss the effect of substrate templating (Dutt *et al.*, EPL 2007), and particle size dispersity (Dutt *et al.*, submitted) on the microstructure of these dense packings, and the macroscopic response to strain. These results use the link between the porosity and internal packing structure via a dynamically tesselating algorithm (Benedict *et al.*, Physica A

2007) which calculates the pore network in dense particulate systems. In addition, we will present some predictions of the macroscopic properties of excipient mixtures from investigations of the material microstructure. We will conclude with some discussions on efforts in modeling pharmaceutical powders by using a combination of DEM numerical experiments and X-ray microtomography imaging.

Signal propagation through dense granular systems. **Lou Kondic** (New Jersey Institute of Technology, USA) IC/MT1214/093

We consider propagation of signals through dense granular systems. The results are obtained by relatively large scale (up to 40,000 particles) discrete element simulations in two spatial dimensions. The properties of the signals are used to deduce the basic physical mechanisms of the force and energy transmission. In addition, we discuss the possibility of developing effective models for signal propagation which bridge the spatial scales between micro (grain scale) and meso (hundreds or thousands of grains) description of granular systems. We also discuss the influence of force anisotropy on the characteristics of the propagating signal. Finally, we will present preliminary results regarding signal propagation through dynamic (sheared) granular system.

IC/MP191/093: Dense granular systems: from theory to applications. #2

Organiser: Lou Kondic (New Jersey Institute of Technology, USA)
Co-organiser: Corey O'Herrn (Yale University, USA)

(For abstract, see session #1 above.)

Jamming, plasticity, and diffusion in dense granular materials. **Robert Behringer** (Duke University, USA) IC/MT1741/093

I will describe recent measurements on systems of photoelastic particles which determine the nature of jamming in a granular material subject to isotropic compression, and then the nature of failure when such a system is subject to shear. Regarding jamming, we obtain data for the pressure , P, the mean contact number per particle, Z, both as functions of the packing fraction, ϕ. We observe a rapid increase in Z as ϕ passes through a critical value. Above ϕ_c, Z and P grow differentially as power-laws in $\phi - \phi_c$ that are in agreement with theory. Regarding plastic failure under shear, we consider the statistical properties of particles within a shear band of a Couette experiment. We consider both locally affine and non-affine behavior. The non-affine displacements characterize local disorder and diffusion, and show gaussian distributions.

Jamming in attractive systems. **Gregg Lois** (Yale University, USA), Corey O'Herrn (Yale University, USA) IC/MT564/093

I will outline recent numerical results on the jamming transition in attractive systems, relevant to cohesive granular materials and powders. As our simulated material is compressed from zero density, we observe three regimes of mechanical behavior that are separated by two second-order critical transitions– percolation and rigidity percolation. This is in contrast to purely repulsive systems that exhibit a single first-order transition. I will give an overview of the mechanical properties in each regime and present measurements of the percolation scaling exponents, which differ from the corresponding lattice values. Although the simulations are athermal, I will demonstrate that the observed behavior also holds for small finite temperatures.

High-density jamming in packings of frictionless aspherical beads. **David Head** (University of Tokyo, Japan) IC/MT1285/093

A convenient, though approximate, means of determining a granular packing's rigidity is to count the number of degrees of freedom of particle motion and constraints of energy invariance, such as fixed interparticle separation. This technique, known as Maxwell counting, seems to give good estimates of rigidity in frictionless spherical and infinite-friction particles. However, the intermediate case of frictionless non-spherical particles has received little attention, perhaps due to a mistaken assumption that it requires non-spherical particles, which are non-trivial to simulate. In fact there is an easier way which is more amenable to efficient simulation, namely to consider spheres of non-uniform mass density such that the particle's centre of mass is displaced from its geometric centre (which still admits non-trivial torque balance equations). Here I will describe initial results from some first simulations employing this approach.

Statistical physics of disordered arrest: from colloidal suspensions to dense granular systems. **Matthias Sperl** (Duke University, USA) IC/MT1622/093

A dense suspension of colloidal hard spheres shows slow and stretched relaxation dynamics over many orders of magnitude in time. It will be shown how this slow dynamics – i.e. the experimental mean-squared displacement – can be fitted and interpreted by a microscopic theory. Changes to the elastic hard-sphere scenario shall be discussed when one introduces (1) attractive interaction, (2) additional soft-core repulsion, and (3) dissipation. Some features found for the dynamics can be used to interpret certain aspects of static granular systems.

IC/MP598/096: Mathematical modeling and numerical analysis of fracture phenomena.

Organiser: Kohji Ohtsuka (Hiroshima Kokusai Gakuin University, Japan)
Co-organiser: Naoshi Nishimura (Kyoto University, Japan)
Co-organiser: Victor Kovtunenko (Universität Graz, Austria)

Mathematical researches on fracture phenomena are of interest to note that the singularity at the edge of cracks generates the crack extension force. The coefficients of singular term are called stress intensity factors in fracture mechanics. This field is constructed of many problems; i.e., crack problems, quasi-static fracture, dynamic fracture, brittle fracture, fatigue fracture, crack path, crack arrest, etc. The purpose of our mini-symposium is to clarify these problems from mathematical viewpoint and to give numerical analysis to simulate fracture phenomena based on mathematical modeling.

However under general situation, crack problem still remain even though crack problem is simplest in this field. Suggested speakers will talk the latest researches on crack problems. In numerical analysis, large scale computations are required for solving complicated fracture problems which include singularities. Latest research results on this topic will be presented by N. Nishimura. In fracture problems, there are many proposals estimating fracture phenomena from mechanical viewpoint.

However, they are independent of each other, and moreover some of them are contradictory. K. Ohtsuka and V. Kovtunenko think that Griffith's energy balance theory will provide basic principle on mathematical modeling of fracture, and Ohtsuka proved that the crack extension force depends only on singularity at the edge of crack in the case of 3-D quasi-static fracture with a crack surface defined by 2-D manifold with the edge under Griffith's principle. In this mini-symposium, we also study Griffith's principle and its modification. Kovtunenko will talk optimization approach to quasi-static crack propagation under non-penetration condition proposed by A. Khludnev.

On inverse crack problems in elastostatics. **Hiromichi Itou** (Gunma University, Japan), Masaru Ikehata (Gunma University, Japan) IC/MT1048/096

In solid mechanics, nondestructive testing has been an important technique in gathering information about unknown cracks, or defects in material. From a mathematical point of view, this is described as an inverse problem of partial differential equations, that is, the problem is to extract information about the location and shape of an unknown crack from the surface displacement field and traction on the boundary of the elastic material. By using the *enclosure method* introduced by Prof. Ikehata we can derive the extraction formula of an unknown linear crack from a single set of measured boundary data. Then, we need to have precise properties of a solution of the corresponding boundary value problem; for instance, an expansion formula around the crack tip. In this talk we will consider the inverse problem concentrating on this point. This research is a joint project with Prof. Ikehata of Gunma University.

Crack detection using topological sensitivity analysis. **Samuel Amstutz** (Université d'Avignon, France), Mohamed Masmoudi (Université Paul Sabatier Toulouse III, France), Imen Horchani (Ecole Nationale d'Ingenieurs de Tunis, Tunisia) IC/MT776/096

The topological sensitivity analysis consists in studying the behavior of a given shape functional with respect a perturbation of the topology of the domain. In general, the nucleation of a small spherical hole is considered. I will show that the concept of polarization tensor allows to extend the analysis to arbitrarily shaped holes and even cracks. Using an appropriate functional, the computation of this sensitivity leads to an efficient and fast method to detect and localize cracks in a domain from boundary measurements. Some numerical experiments in this context will be presented.

IC/MP598/096: Mathematical modeling and numerical analysis of fracture phenomena. #2

Organiser: Kohji Ohtsuka (Hiroshima Kokusai Gakuin University, Japan)
Co-organiser: Naoshi Nishimura (Kyoto University, Japan)
Co-organiser: Victor Kovtunenko (Universität Graz, Austria)

(For abstract, see session #1 above.)

Mathematical modeling of stable quasi-static crack extension by extended Griffith energy-balance theory. **Kohji Ohtsuka** (Hiroshima Kokusai Gakuin University, Japan) IC/MT931/096

Griffith's approach to fracture mechanics is very powerful, and there are many extensions and modifications of Griffith's work. Here, upon Griffith's idea, we derive a *criterion for stable and unstable crack extension* of a crack with the shape of arbitrary surface Σ with the edge $\partial\Sigma$ in three-dimensional solids subjected to arbitrary loads. The crack extension process is considered to occur in a quasi-static manner such that inertial effects may be neglected. Therefore, when we refer to time t we use it as a parameter that delineates the history of sequence of events such as loading $\mathcal{L}(t)$ and crack extension $\Sigma(t)$. Under a loading $\mathcal{L}(t)$, if a virtual crack extension $\{\Sigma(t)\}$ is given in the form of the sequence of surfaces with the edge, then we can get the displacement vector as the weak solution of the variational problem defined on $\Omega_{\Sigma(t)} = \Omega \setminus \Sigma(t)$. Here Ω denotes the bounded domain with smooth boundary and is assumed satisfying $\Sigma(t) \subset \Omega$. Griffith's energy balance theory is so that it is applicable only when $\mathcal{L}$ remains constant during crack extension. However, in general, the released energy increases as long as $\mathcal{L}$ remains constant. For this, to consider the stopping of crack extension, we need the modification for the energy release rate to be applicable under varying loads. With this modification, driving new formula $\mathcal{F}_{\Sigma(\cdot)}(t)$, we can extend Griffith's energy balance theory in consideration of second expansion of energies and crack extension resistance with respect to time. We now define that $\Sigma(t)$ is *unstable*, if $\mathcal{F}_{\Sigma(\cdot)}(t) > 0$ for all $t > 0$. We can also derive the criterion of stability.

Quasi-static evolution in brittle fracture based on local minimization. **Christopher Larsen** (Worcester Polytechnic Institute, USA) IC/MT3904/096

Based on Griffith's criterion for crack growth, a method was recently proposed for determining crack paths by taking continuous-time limits of discrete-time variational problems. This has been successfully carried out, but an important difference remains between these solutions and Griffith's model. I will explain the method and the main issues in its implementation, and then describe the remaining gap and some efforts to remove it.

Optimization in constrained crack problems. **Victor Kovtunenko** (Universität Graz, Austria), Alexander Khludnev (Lavrentyev Institute of Hydrodynamics, Russian Federation) IC/MT633/096

Following the optimization approach to brittle fracture, we consider evolution of a crack in a domain as solution of the global problem of minimization of the total potential energy with respect to shape variables. For instance, the shape optimization problem is well-posed with respect to the length-parameter of the crack, that describes its quasi-static propagation by delamination process.

The necessary ingredients include:

Kinematic description of crack evolution by given a-priori vector of the velocity field can be given in two ways: constructing one-to-one coordinate transformation between domains with cracks with the help of nonlinear ODE, or by implicit surfaces solving a linear transport equation.

Modeling of equilibrium of solids with crack is given in the framework of variational formulation of the static problem, accounting conditions of non-penetration between the crack surfaces in the admissible set, which results in constrained crack problems.

The primal-dual shape sensitivity technique of is applied to describe kinematic characteristics of the crack problems with respect to regular perturbations of parameters of the crack shape with given velocity vector field, in particular, to find the energy release rate at the crack tip by means of the first directional derivative.

For numerical optimization, based on the generalized differentiability property, a semi-smooth Newton method is proposed

in the form of primal-dual active-set methodin as the efficient numerical technique for solution of constrained minimization problems, in particular with cracks, due to the property of its unconditional global and, moreover, monotone convergence.

The global optimization is realized in a constructive way on the set of extremal points of the cost functional by the path-following methods, which use the differentiability property of the reduced energy function. Numerical examples present quasi-static propagation of cracks during the delamination process in composite, based on the refinement of the Griffith fracture law in frame of the optimization approach.

Dynamical crack propagation in a 2D elastic body, the out-of-plane state. **Anna-Margarete Sändig** (Universität Stuttgart, Germany), Serge Nicaise (Université de Valenciennes, France), Adriana Lalegname (Universität Stuttgart, Germany) IC/MT981/096

We discuss the propagation of a running crack under shear waves in a rigorous mathematical way for a simplified model. This model is described by two coupled equations in the actual configuration: a two-dimensional scalar wave equation in a cracked bounded domain and an ordinary differential equation derived from an energy balance law. The unknowns are the displacement fields $u = u(y,t)$ and the one-dimensional crack tip trajectory $h = h(t)$. We handle both equations separately, assuming at first that the crack position is known. Existence and uniqueness of strong solutions of the wave equation will be studied and the crack-tip singularities will be derived under the assumption that the crack is straight and moves tangentially. Using an energy balance law and the crack tip behaviour of the displacement fields we finally arrive at an ordinary differential equation for $h(t)$, called equation of motion for the crack tip. We demonstrate the crack-tip motion with the corresponding nonuniformly crack speed by numerical simulations.

IC/MP201/096: Computational aspects in finite electro- or magneto-elasticity.

Organiser: Paul Steinmann (TU Kaiserslautern, Germany)
Co-organiser: Gérard Maugin (Université Pierre et Marie Curie, France)

In the recent years various novel materials have been developed that respond mechanically to the application of electrical or magnetical loading by large strains. Examples are the classes of so-called electro-active and magneto-sensitive polymers. Certainly these materials are technologically very interesting; e.g., for the design of actors in mechatronics or in the area of artificial soft tissue biomechanics.

The minisymposium thus focuses (i) on the modelling of electro- and magneto-elastic materials within the setting of geometrically nonlinear continuum-electro-dynamics (often spezializable to the case of electro- or magneto-elasto-statics) and (ii) in particular to the corresponding computational setting. Thereby a highly nonlinear coupled problem for the deformation and the electric or magnetic (scalar or vector) potential has to be solved, that is only amenable to computational solution techniques.

As an interesting and probably less known aspect the minisymposium highlights also the theoretical and computational treatment of various defects (like e.g., cracks or inclusions), for this example of a coupled multiphysics problem. The study of configurational continuum physics renders a valuable tool for the analyst in order to examine further properties of the solution which would otherwise be hidden.

Simulation of poly-crystalline ferro-electrics based on discrete orientation distribution functions. **Jörg Schröder** (Universität Duisburg-Essen, Germany) IC/MT2154/096

Ferro-electric materials can be found in a wide range of applications in smart materials; e.g., vibration reducing sensors or fuel injection systems. A special characteristic feature of these materials is the appearance of a spontaneous polarization in a certain temperature range. This polarization can be reversed by an applied electric field of sufficient magnitude. The resulting nonlinear material behavior is expressed by characteristic dielectric and butterfly hysteresis loops. In case of single crystals these effects are correlated to the structure of the crystal and especially to the axis of the spontaneous polarization.

The anisotropic material behavior is modeled within a coordinate-invariant formulation for an assumed transversely isotropic material, see [1,2]. The anisotropic response of the material is governed by isotropic tensor functions which depend on a finite set of invariants. In order to model the nonlinear material behavior a switching surface is defined and evolution equations for the remanent quantities are derived. For the consideration of the polycrystalline material behavior we start with a representative meso scale, where the domains consist of unit cells with equal spontaneous polarization. The main equations of the mesoscopic boundary value problem are the balance of momentum and the Gauss law respectively. For the derivation of the boundary conditions on this scale we consider a generalized macrohomogenity condition which equates the macroscopic and the mesoscopic electromechanical work. In this investigation we obtain the macroscopic polycrystalline quantities via a simple homogenization procedure, where discrete orientation distribution functions are used to approximate the different domains. The resulting hysteresis loops for a ferroelectric ceramic are discussed and some numerical examples are presented.

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[2] Schröder, J. & Romanowski, H.; A thermodynamically consistent mesoscopic model for transversely isotropic ferroelectric ceramics in a coordinate-invariant setting, Archive of Applied Mechanics, **74**, 863–877, 2005.

Numerical simulation of electro- and magneto-elasticity. **Duc Khoi Vu** (TU Kaiserslautern, Germany), Paul Steinmann (TU Kaiserslautern, Germany), Gunnar Possart (TU Kaiserslautern, Germany) IC/MT3327/096

Electro- and magneto-sensitive elastomers belong to the class of smart materials that exhibit large displacement and change their mechanical behavior in response to the application of electric or magnetic fields and have been the subject of many researches in the last few years due to their interesting application including robotic arms that are actuated by artificial muscles, adaptive tuned vibration absorbers, stiffness tunable mounts and suspensions and automotive bushing, see for example [1-5].

Besides the various difficulties facing researchers in their effort to produce effective systems driven by electro or magneto-sensitive elastomers, due to their nonlinear electro- and magneto-mechanical coupling behavior the modelling and simulation of these materials is also a challenging task. The governing equations and some simulations of the electroelastic and magnetoelastic coupling problems were addressed in [5-9]. Based on these previous studies, the numerical simulation of nonlinear electro- and magneto-elasticity is addressed

in this work.

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[2] Kordonsky, W., 1993: Magneto-rheological effects as a base of new devices and technologies. J. Mag. Mag. Mater. 122, 395–398.

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[4] Jolly, M. R., Carlson, J. D., Munoz, B. C., 1996. A model of the behavior of magneto-rheological materials. Smart Mater. Struct. 5, 607–614.

[5] Dorfmann, A., Ogden, R.W., 2004. Nonlinear magnetoelastic deformations of elastomers. Acta Mechanica 167(1-2), 13–28

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[8] Brigdanov, I.A., Dorfmann, A., 2003. Mathematical modeling of magneto-sensitive elastomers. Int. J. Solids Struct. 40 (18), 4659–4674

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The mechanics of interfaces between elastic dielectrics and application towards cracks in piezoelectrics. **Andreas Ricoeur** (TU Bergakademie Freiberg, Germany), Meinhard Kuna (TU Bergakademie Freiberg, Germany) IC/MT4030/096

Interfaces between dielectric solids can be found in laminated structures or composite materials. Dielectric interfaces are also present at the boundaries between solid bodies and fluids or a vacuum. Likewise, the faces of a crack in a dielectric material are interfaces between a solid and vacuum, air or an insulating liquid. If either an electric load is imposed on the aforementioned systems or the bodies exhibit physical properties coupling mechanical and electrical fields, forces and related displacements are induced at the interfaces as well as inside the body. Although sometimes small compared to the effect due to mechanical loads, these forces should be included into a comprehensive analysis of the mechanics of dielectrics.

The theoretical background is based on thermodynamical considerations of linear dielectrics and piezoelectrics including inhomogeneities and defects. Material or configurational forces are calculated from the explicit space-variance of thermodynamical potentials. The forces acting on an interface are derived likewise, introducing the MAXWELL tensor of electrostatics. Here, different approaches are discussed. The results are applied to cracks in piezoelectric ceramics. Considering the crack slit as a medium of finite dielectric permittivity, the boundary conditions on the crack faces are formulated both dielectrically and thermodynamically consistent. Calculating the J-Integral, crack surface loads have to be taken into account. In doing so, the classical contour integration is replaced by a simple jump term. Depending on the modeling of the crack faces, i.e. electrical and mechanical boundary conditions, the approach is only exact for arbitrary cracks if a simplified model for crack surface tractions is applied. In all other cases it is shown to be a good approximation. The influence of different crack face boundary conditions on fracture mechanics quantities is demonstrated by means of analytical examples.

IC/MP201/096: Computational aspects in finite electro- or magneto-elasticity. #2

Organiser: Paul Steinmann (TU Kaiserslautern, Germany)
Co-organiser: Gérard Maugin (Université Pierre et Marie Curie, France)

(For abstract, see session #1 above.)

Continuum thermodynamic modeling and simulation of electromagnetic metal forming processes. **Bob Svendsen** (Universität Dortmund, Germany), Jaan Unger (Universität Dortmund, Germany) IC/MT2321/096

The purpose of this work is the formulation and application of a continuum thermodynamic approach to the phenomenological modeling of a class of engineering materials which can be dynamically formed using strong magnetic fields. This is carried out in the framework of a thermodynamic, internal-variable-based formulation in which the deformation, temperature and magnetic fields are in general coupled. This coupling takes the form of the Lorentz force as an additional supply of momentum, and the electromotive power as an additional supply of energy, in the material. In the current approach, the basic thermomechanical field relations for mass, momentum and moment of momentum are obtained from the total energy balance via invariance, and completed by Maxwell's field equations. The constitutive formulation is based on the exploitation of the Müller-Liu entropy principle, here for the case of isotropic thermoelastic, viscoplastic material behaviour. The resulting reduced constitutive and field relations and restrictions are then applied to the modeling and simulation of high-speed electromagnetic forming of metal tubes and sheet metal. The finite-element numerical simulation here is based on a staggered solution scheme involving a Lagrangian mesh and stabilized solid-shell elements for the workpiece together with an ALE-based formulation utilizing Nédélec elements for the electromagnetic part of the problem. Simulation examples will be presented.

A variational formulation for magneto-active elastomers based on the total-energy approach. **Roger Bustamante** (University of Glasgow, UK) IC/MT1611/096

This presentation focuses on variational formulations of a magneto-active elastomer completely surrounded by free (vacuum) space [1]. The free space is considered finite, with an applied magnetic field or magnetic induction vector as the far field boundary conditions. The entire surface of the body is in direct contact with the free space, additionally a mechanical load is applied over a portion of the surface. No displacement constraints are considered.

For this boundary value problem two equivalent variational formulations are proposed, which are formulated in terms of the *total energy function* Ω introduced by Dorfmann and Ogden [2,3]. One of these formulations is based on the use of the displacement field and the magnetic scalar potential (for the magnetic field), the second equivalent formulation is based on the magnetic vector potential (for the magnetic induction) in addition to the displacement.

Important questions regarding the use of the *Maxwell stress* for the boundary conditions are discussed.

[1] R. Bustamante, A. Dorfmann and R. W. Ogden; A variational formulation for the traction problem for magneto-active elastomers. *In preparation*.

[2] A. Dorfmann, R. W. Ogden; Nonlinear magnetoelastic deformations. Q. Jl. Mech. Appl. Math. **57** (2004), pp.599–622.

[3] A. Dorfmann, R. W. Ogden; Nonlinear magnetoelastic deformations of elastomers. Acta Mechanica **167** (2004), pp.13–28.

Equivalent governing equilibrium equations for nonlinear magneto-elastic solids. **Luis Dorfmann** (Tufts University, USA), Roger Bustamante (University of Glasgow, UK) IC/MT2244/096

In recent years there has been considerable renewed interest in electromagnetic theories of materials capable of large elastic deformations. This is motivated by the need for accurate constitutive equations to support the use of so called 'smart' materials for the development of a number of industrial devices.

The theoretical foundations for a continuum deforming in the presence of an electromagnetic field are given, for example, by Truesdell and Toupin [9], Brown [1], Eringen and Maugin [5] and Kovetz [7]. More recent theoretical works are those by Steigmann [8], Kanakanala and Triantafyllidis [6], Dorfmann and Ogden [3,4] and Bustamente *et al.* [2].

In this presentation we give an overview and evaluate alternative formulations of the governing equilibrium equations for nonlinear magnetoelastic deformations of magneto-sensitive solids. We highlight differences (but in principle equivalent) formulations and show possible restrictions imposed by the magnetic field equations on the form of the constitutive laws. In particular, we provide a detailed comparison of our formulation with the one given by Steigmann [8], Kanakanala and Triantafyllidis [6] and Brown [1].

[1] W.F. Brown, *Magnetoelastic Interactions* (Springer, Berlin 1966).

[2] R. Bustamante, A. Dorfmann and R. W. Ogden, A variational formulation for the traction problem of magneto-active elastomers. *In preparation.*

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Surface stability of nonlinear magneto-elastic solids. **Melanie Ottenio** (Université Bordeaux I, France) IC/MT3283/096

Nonlinear magnetoelastic solids offer interesting industrial applications because their damping abilities can be tuned by adequate outside magnetic fields. Here, we propose to derive the equations governing the deformations of infinitesimal disturbances superimposed onto large static fields in magnetoelasticity. The coupling between the equations of mechanical equilibrium and Maxwell's equations complicates the formulation of incremental elasticity. However, our approach is based on Dorfmann and Ogden's work, which allows to obtain the governing coupled equations in a form similar to the form of the governing equations of nonlinear elasticity. Then, we propose to look for the conditions of surface stability when the solid is held in plane strain and a magnetic induction vector is applied along the normal to the surface. How large can be the applied magnetic field and how much can we pre-strain the half-space before reaching the bifurcation criterion are the questions that we try to answer.

09: Solid Mechanics, Contributed Talks

IC/CTS4622/09: **Material interfaces, composites, microstructure, smart materials.**

Organiser: David Natroshvili (Georgia Institute of Technology)

A kinetic Monte-Carlo study illustrating control of morphological instability during directional epitaxy. **Michael Saum** (University of Tennessee, USA), Tim Schulze (University of Tennessee, USA) IC/CT2514/092

We consider a Kinetic Monte Carlo (KMC) model of directional epitaxy for both single and multi-species growth. In particular, we present a model for the continuous processing of thin film deposition on a moving substrate. Instabilities in the morphology of the resulting surface are initiated by the presence of the Erhlich-Schwoebel barrier and result in the self assembly of structures with different characteristics. We illustrate how these morphological changes can be controlled by varying parameters such as temperature, the substrate pulling velocity, and deposition flux profile.

Gradient second-order interphase-layer theory of continuous media with micro-structures. **Sergey Lurie** (Russian Academy of Sciences, Moscow), Natalia Tuchkova (Russian Academy of Sciences, Moscow) IC/CT917/092

The interphase layer theory is developed on the base of the continuum media with conserved dislocations [1]. The rigorously formulated continuous media models with microstructure are proposed. Correctness of the developed models is justified by application of the kinematic variational principle based on the consistent formal description of the media kinematics and formulation of the kinematic relations for the media of a different complexity, as well as on the construction of the relevant potential strain energy with the use of the Lagrangian multipliers procedure. The special attention is paid to the analysis of kinematic relations since in the framework of variational description the kinematics of medium fully defines the system of internal volumetric and surface interactions of the body under study. The set of constitutive relations is derived and the corresponding consistent boundary-value problems are formulated. For the first time, the interpretation of all physical characteristics that are responsible for non-classical effects is proposed, and the entire spectrum of adhesion mechanical parameters is described. The general model of continuous media proposed in the present paper is a first rigorous theoretical model that allows to analyze various particular scale effects, e.g., cohesive interactions, surface effects (surface tensions, wettability, capillarity etc.) both in the volume and on a surface within the unified continuum description. By the model it was found that these effects could help to understand-predict macro-micro mechanics of the material, if the boundary conditions and phase effects are modeled across the length scales. The prediction methodology and modeling tools have been developed for numerical simulations and analysis of the stress-strain-stress and mechanical properties across the length scales [2-5]. 1. Lurie, S. and Kalamkarov, A Int. J. Solid and structures,2005, 43(1). 2. Lurie, S. et al. 2003 In: Analysis and Simulation of Multifield Problems, Springer, 12. 3. Lurie, S. et al. 2003. Int J Comp Mater Scs, 3-4.. 4. Lurie, S.et al. 2005. Int. Journal "Computational Materials Science" A., 36(2). 5. Volkov-Bogorodsky D., Lurie S, et al. 2006. Comput. Math. and Math. Phys., 46(7).

Mathematical problems for piezoelectric–metallic composites. **David Natroshvili** (Georgia Institute of Technology) IC/CT1069/092

We study the following mathematical problem related to engineering applications: Given is a three-dimensional composite consisting of a piezoelectric (ceramic) matrix with metallic inclusions (electrodes). We derive a linear model for the interaction of the corresponding 4-dimensional thermoelastic field in the metallic part and 5-dimensional thermoelectroelastic field in the piezo-ceramic part.

The main difficulty in the modelling is to find appropriate boundary and transmission conditions for the composed body. The mathematical analysis includes then the study of existence, uniqueness and regularity of the resulting elliptic boundary-transmission problem assuming the metallic and ceramic materials occupy smooth or polyhedral domains.

With the help of the indirect boundary integral equations method we reduce the complex transmission problem to the equivalent strongly elliptic system of pseudodifferential equations involving pseudodifferential operators on manifold with boundary. The solvability and regularity of solutions to these boundary integral equations and the original transmission problem are analyzed in Sobolev-Slobodetski (Bessel potential) H^s_p and Besov $B^s_{p,t}$ spaces. This enables us to investigate also stress singularities which appear near zones, where the boundary conditions change and where the interface meets the exterior boundary. We show that the order of the singularity is related to the eigenvalues of the symbol matrices of the corresponding pseudodifferential operators and study their dependence on the material constants of the composite.

Nanoscale modeling of the elastic contact between a rigid indenter and an elastic half-space. **Dan Dumitriu** (Institute of Solid Mechanics, Romania) IC/CT484/092

In the theory of elasticity, mixed boundary value problems arise naturally in elastic contact problems. This paper deals with the elastic contact between a rigid indenter of known tip geometry and an elastic half-space. Indentation is a method used to analyse the characteristics of materials related to different mechanical processes, such as: fracture, defect nucleation, adhesion, friction, wear. Here the indentation problem is studied at the nanometric scale, where classical continuum mechanics can no more accurately model the elastic contact. New coupled atomistic–continuum methods must be used to solve the elastic nanocontact problem.

At the nanometric scale, EringenŠs nonlocal theory describes better than classical (local) continuum mechanics methods the long-range interactions among the particles in materials. In the classical theory, the balance laws are valid for every part of the body, no matter how small it may be, and the localization condition yields to the vanishing of integrants in the integrals. In the nonlocal theory, this assumption is abandoned, but the localization is still possible with the aid of certain localization residuals, which must integrate to zero. These residuals are the effects of all other points of the body on one point of the body, that means the residuals are the long-range effects of all points at which the balance laws are localised.

The nonlocal formulation is numerically solved using a finite elements code written in C. One has to solve a linear equations system of big dimensions, without dealing with a sparse matrix as in local approaches.

The nanoindentation example presented in the paper concerns a flat punch of arbitrary shape. For parabolic, circular, elliptic and square punches, closed form exact solutions for contact pressures and penetration are obtained, using SneddonŠs dual integral equations. The contact pressures are bounded and continuous functions inside and on the boundary of the contact domain. The availability of exact solutions for these particular flat punches permits to validate the proposed numerical resolution of the nonlocal formulation. Once the numerical code validated, it can be used for any arbitrary shape of the flat punch.

Materials with inter- and intralaminar defects under in-plane compression. **Igor Guz** (University of Aberdeen, UK), Maria Kashtalyan (University of Aberdeen, UK) IC/CT1169/092

Various types of inter- and intralaminar defects may occur in layered materials during the fabrication process or in-service. Interlaminar defects include cracks, zones of non-adhesion, reduced adhesion and slippage, and similar imperfections, while intralaminar defects could be cracks, voids, porosity etc.

When a layered material is compressed along the layers, fracture due to interlaminar defects cannot be predicted using the classical Griffith-Irwin criterion or its generalisations, and therefore fracture due to mechanisms, specific to heterogeneous materials, needs to be considered. One of such mechanisms is internal instability, i.e. the loss of stability in the microstructure of the heterogeneous material. Here the internal instability of non-linear layered materials with inter- and intralaminar defects undergoing finite (large) deformations is investigated. For cleavage-type delaminations, the upper and the lower bounds for critical load are established. The bounds are based on the exact analytical solutions for 3-D problems considered within the model of piecewise-homogeneous medium.

The presence of intralaminar defects is accounted for by replacing the layers with defects with equivalent homogeneous ones with appropriate effective properties. To take account of the in-situ constraint of the neighbouring layers on the effective properties of a particular layer with defects, it is suggested to use the Equivalent Constraint Model of the damaged layer. Previously, the model was successfully used to predict effective properties of cracked layers in fibre-reinforced composite laminates.

The effect of the different types of inter- and intralaminar defects, layer thickness and stiffness on the lower and the upper bounds is examined for a number of non-linear models of materials under various kinds of loading. The obtained results show that the bounds present a good estimation.

Newton's coefficient of restitution at the macro- and nano-scales. **Graham Weir** (Industrial Research, Ltd., New Zealand) IC/CT2077/095

Newtons Coefficient of Restitution, for low velocity impacts between macroscopic rigid-plastic identical spherical particles, depends primarily on the initial relative velocity, Youngs Modulus, particle size and the plastic yield stress. Surface tension becomes important for impacts between nano-scale particles. The major implications of surface tension for impacts at the nano-scale are discussed, and some approximations are possible by referring the nano-scale parameters down to the atomic scale. New results are presented on the order of magnitude for the yield strength of nano-scale material particles.

IC/CTS4629/09: Theoretical topics incl. granular material.

Analysis and simulation of dune evolution: from a dynamical-system perspective. **Serina Diniega** (University of Arizona, USA), Karl Glasner (University of Arizona, USA) IC/CT3028/093

Dunes are common landforms, developing whenever there is a source of granular material, wind of sufficient strength to move this material, and an "obstacle" to induce initial accumulation. They have been found on Earth, Mars, and Titan.

The aim of this research is to formulate a simple BCRE-type model of dune genesis, behavior, and morphology, through numerical simulation and Dynamical Systems analysis. Currently, the model considers a two-dimensional dune field. Coupled partial differential equations govern the exchange of sand between a "static sand" layer (the dune) and a "moving sand" layer. In the equations, simple functions average together the sand transport processes (saltation, reptation, creep) to yield erosion and deposition amounts. The moving layer advects, and diffusion terms account for smoothing processes (air turbulence, avalanching).

Standard Dynamical Systems analysis has been done to nondimensionalize the equations, determine stability about the steady-state system (flat plane of sand with constant flux), and find characteristic scalings of the system. With reasonable parameter values, long-wavelength instabilities were found. These instabilities are the cause of the formation and growth of dune-type structures.

The model has also been numerically simulated, through a two-step process which considers the uncoupled nonlinear parts first. Initial conditions were chosen as random perturbations about the steady-state solution, and periodic boundary conditions were employed to keep the total mass of the system constant. Both random and sinusoidal initial conditions were found to quickly coalesce into a few piles of sand, which moved across the simulation box. As the simulation progressed, the piles continued to coalesce until one large pile of sand remained and moved at a uniform speed across the simulation box.

Numerical analysis of micro-stress evolution in dual-face polycrystals. **Jan Ocenasek** (TU München, Germany), Christian Krempaszky (TU München, Germany) IC/CT3624/009

Wide range of mechanical and thermal treatments of materials and components are commonly applied to obtain characteristic mechanical properties. Identification of macroscopic residual stresses caused by those treatments is essential to prevent undesirable distortion of further machined components or to predict reliably the stress state of parts during working time.

Neutron diffraction brought several advantages in investigation of residual stresses, but its application is limited for example by finite size of excited volume or by microstructural features of investigated material like multiface structure, texture, grain size, precipitations and upcoming interphase and intergranular microstresses. In literature experimental results that are not consistent with considerations of mechanical equilibrium have been explained up to now by assuming nonhomogeneously distributed and anisotropic lattice parameters [Dye D. et al., Metall. and Mat. Transactions 2004].

A numerical study analysing the evolution of stresses in polycrystalline microstructure under several loading conditions is presented. The aim of this study is to better understand the impact of intergranular and interphase stresses on diffraction-based residual stress analysis.

Computer simulations based on representative volume element using periodic boundary conditions (to reduce high computational costs) are presented. Particular grains follow the continuum crystal plasticity constitutive law to capture both elastic and plastic anisotropy of single crystals structures. Voronoi tessellations are used to mimic real spatial morphology of polycrystals. Results are discussed together with experimental data of neutron diffraction measurements.

Newton-like solver for elastoplastic problems with hardening and its local super-linear convergence. **Peter Gruber** (Universität Linz, Austria), Jan Valdman (Universität Linz, Austria) IC/CT3030/096

We discuss a solution algorithm for quasi-static elastoplastic problems with linear hardening. After discretization in time, such problems can be discribed by the minimization of a functional, which depends on the plastic strain non smoothly, and on the displacement and a hardening parameter smoothly. For the most relevant models of hardening, the minimizers for the plastic strain and the hardening parameter can be calculated explicetely. By substitution, one obtains a minimization functional which depends on the displacement only.

A theorem of J. J. Moreau from convex analysis states, that this functional is differentiable and the derivative can be computed explicitely. This is a non trivial result, since the original functional depends non smoothly on the plastic strain, and the plastic strain minimizer depends non smoothly on the displacement.

However, the second derivative of the energy functional does not exist. As a remedy, we utilize a concept of slanting functions, which was recently developed by X. Chen, Z. Nashed and L. Qi. A Newton-like method, exploiting slanting functions of the energy functional's first derivative, is proposed. The local super-linear convergence of this method is shown in the FE-discrete case, and sufficient regularity assumptions are formulated, which imply the local super-linear convergence also in the spatially continuous case.

Time integration of inelastic material models exhibits an order reduction for higher-order methods - can this be avoided?. **Charlotte Kuhn** (TU Darmstadt, Germany), Bernhard Eidel (TU Darmstadt, Germany) IC/CT2302/096

For the numerical treatment of inelastic material behavior within the finite element method a partitioned ansatz is standard in most of the software frameworks; the weak form of equilibrium is discretized in space and solved on a global level, whereas the initial value problem for the evolution equations of internal state variables is separately solved on a local, i.e. Gauss-point level, where strains, derived from global displacements, serve as input, [1].

Applying higher order methods ($p > 2$) to the time integration of plasticity models, an order reduction is reported, where Runge-Kutta schemes have shown hardly more than order two at best, [2].

In the present contribution, we firstly analyze for the ODE case of viscoelasticity the reason for order reduction and in doing so focus on the crucial role of strain approximation for multi-stage methods in time integration. Next, we extend our considerations to the DAE case of plasticity, where the switching point detection must additionally be considered for the generation of consistent initial data. We specify our general procedures for both types of constitutive behavior to Runge-Kutta methods of Radau IIa class and show their improved performance in representative numerical examples.

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Configurational forces in a micro-cracked body. **Malika Bongué Boma** (Laboratoire Central des Ponts et Chaussées, France), Maurizo Brocato (École Nationale Supérieure d'Architecture de Versailles, France) IC/CT4380/096

A model assessing the behaviour of a micro-cracked body under slow mechanical loading is presented.

Calling upon the theory of microstructure, the kinematics of the domain is enriched thanks to a variable characterising size and orientation of the crack field. Balance equations and boundary conditions governing the evolution of its dual variables are determined.

The crack field can propagate following the macromotion i.e. the latent microstructure is determined by the macroscopic gradient of deformation. However we deal with a configurational evolution that changes the integrity of the body: considering a non dissipative movement, the crack doesn't recover its initial size after load removing.

We therefore divide the evolution of the body in two fictive evolutions:

- Propagation of the micro-cracks: the body evolves from the reference configuration to an intermediate one without any movement of its material points. We hence define a configurational parameter characterising the propagation velocity of the crack field.
- Deformation of the body: it evolves from the intermediate to the current configuration following the macromotion.

We determine the new balance equations and boundary conditions governing those two evolutions. Some new stresses appear in the model. They will be called micro-configurationnal because they are configurational forces associated to a microstructural variable. Those four stresses are dual to the first and second gradient of deformation and dual to the the crack propagation parameter and its gradient.

IC/CTS4619/09: Modelling of nonlinear systems.

Organiser: Doina Liana Pisla (Universitatea Tehnicã Cluj-Napoca, Romania)

Non-local boundary-value problem for a system of singular differential equations and applications to cusped prismatic shells. **George Jaiani** (Tbilisi State University, Georgia) IC/CT4427/015

The paper deals with a system of singular partial differential equations of the first and second order arising in the zero approximation of I.Vekua's hierarchical models of prismatic shells [1], when the thickness of the shell varies as a power function of one argument and vanishes at the cusped edge of the shell [2], [3]. For this system of special type a nonlocal boundary value problem in a half-plane is solved in the explicit form. The boundary value problem under consideration corresponds to stress-strain state of the cusped prismatic shell under the action of concentrated forces and moments.

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Deformations of wrinkled fiber-reinforced membranes. **Elena Shmoylova** (Tufts University, USA), Luis Dorfmann (Tufts University, USA) IC/CT4507/015

In this presentation we discuss wrinkling of non-linearly elastic membranes. Some aspects of this phenomenon for isotropic and anisotropic membranes have been investigated in the past and results are available in the literature. However, the development of wrinkled regions in non-linearly elastic membranes reinforced with one or two families of fibers, to the best of our knowledge, has not been investigated.

We consider the modeling of wrinkling of non-linearly elastic membranes as an initial step to improve our understanding of the development and the structural response of many biological and native tissues, for example, wrinkling formation in the human skin. Since most biological tissues have a complex anisotropic structure and often contain naturally formed fibers (e.g. collagen fibers), fiber-reinforced membranes deserve special attention.

We determine wrinkled regions for different geometric layouts, which can be described by the membrane theory. The objective of the work is to determine optimal fibers' orientation that minimizes the wrinkled regions for given boundary conditions. Also, we show that for selected geometric configurations and given boundary conditions, a fibers' orientation may be found which has no effect on the overall wrinkle formation, i.e. the structural response is not influenced by the presence of the reinforcing fibers. We believe that these findings may provide an interpretation of how and why some native fiber-reinforced tissues grow and remodel.

Buckling of a spherical shell embedded in an elastic substrate with a uniaxial stress field at infinity. **Gareth Jones** (University of Oxford, UK), Jon Chapman (University of Oxford, UK), David Allwright (University of Oxford, UK) IC/CT4759/015

For many underwater applications, tiles made of a certain composite material are used to minimise the reflection coefficient of submerged bodies. This material consists of a rubber substrate, containing gas-filled microspheres which are a few microns in diameter. In their application, the tiles are compressed uniaxially, which induces a uniaxial stress field in the material. This will cause the embedded shells to buckle, thus softening the material. To examine this phenomenon we consider the linear elastic problem of an isolated embedded shell, with a uniaxial stress field at infinity in the substrate. The critical stress for buckling is determined by the Rayleigh–Ritz method, expanding the buckled shell displacement in a series of Legendre functions. This numerically-determined critical stress is then examined in the limit as the thickness ratio of the shell tends to zero, with the aid of WKB analysis. We obtain analytic expressions for the critical stress and buckling pattern in this limit.

On kinematics of a parallel robot used for the minimally-invasive surgery. **Doina Liana Pisla** (Universitatea Tehnicã Cluj-Napoca, Romania), Nicolae Plitea (Universitatea Tehnicã Cluj-Napoca, Romania), Calin Vaida (Universitatea Tehnicã Cluj-Napoca, Romania), Adrian Pisla (Technical University Cluj-Napoca, Romania) IC/CT807/095

Robotic systems have been developed in every field where a further progress was constricted due to the human limitations in terms of speed, precision, fatigue, repeatability, strength, etc. Parallel robots offer a higher stiffness and smaller mobile mass than serial robots, thus they allow faster and more precise manipulations. The problems concerning parallel structures kinematics are usually more complicated than for the serial structures. One of the pioneer fields for robots is their assimilation in surgery, especially in minimally invasive procedures which aim the treatment of a disease with minimum damage to healthy tissue and suffering for the patient. The paper presents the geometric and kinematic model of an innovative parallel structure for the manipulation of surgical instruments in minimally invasive surgery. The parallel architecture

has been chosen for its superiority in precision, repeatability, stiffness, higher speeds and occupied volume. Another important feature is the smaller working volume of such a structure, which in this case is a supplementary safety measure, which is provided by the structure itself. The equations, which model the geometric and kinematic models, are pointed out for this robot based on its mathematically determined functional parameters. The results of the kinematical modeling are systematically presented and lead to the facile solving of the parallel structure.

For this new structure the authors will develop a haptic feedback system which will eliminate the one of the biggest complains of the doctors referring to the lack of tissue feeling.

This system will allow doctors, which manipulate the robot to actually feel the resistance of the tissues and organs of the patient thus having a second control besides the visual one. The cheaper structure will allow a wider spread or the robot in the operation room an easier acceptance and a better feedback for further improvements. Some simulation results have been presented.

Stress distribution around a crack in plane micropolar elasticity. **Stanislav Potapenko** (University of Waterloo, Canada) IC/CT3965/094

The theory of micropolar elasticity (also known as Cosserat or asymmetric theory of elasticity) was introduced by Eringen to eliminate discrepancies between classical theory of elasticity and experiments in cases when effects of material microstructure were known to contribute significantly to the body's overall deformation, for example, materials with granular microstructure such as polymers or human bones. These cases are becoming increasingly important in the design and manufacture of modern day advanced materials as small-scale effects become very important in the prediction of the overall mechanical behavior of these materials.

In this presentation we use the boundary element method to find the solution for an infinite domain weakened by a crack in plane Cosserat elasticity, when stresses and couple stresses are prescribed along both sides of the crack (Neumann boundary value problem), and discuss its convergence. To illustrate the effectiveness of the method for applications we consider a crack in a human bone which is modelled under assumptions of plane micropolar elasticity. We find the numerical solution for stresses around the crack and show that the solution may be reduced to the classical one if we set all micropolar elastic constants equal to zero. We come to the conclusion that there could be up to 26 percent difference in quantitative characteristics of the stress around a crack in the micropolar case in comparison with the model when microstructure is ignored.

Analytical solution to the problem of adhesive elastic contact of a sphere with a substrate. **Olesya Zhupanska** (University of Florida, USA) IC/CT3527/015

The renewed interest in adhesive contact problems is associated with the development of advanced measurement techniques, i.e. atomic force microscopy, nanoindentation, which enable testing of mechanical properties of materials at the nanometer scale. Interpretation of some of the measurement results is a challenging problem and is still under discussion. The problem is partially attributed to adhesion of contacting surfaces that influence contact interaction between the instrument tip and tested material surface. The most widely recognized adhesive contact models, i.e. JohnsonŰKendallŰRoberts (JKR) and DerjaguinŰMullerŰToporov (DMT) take into account only the transmission of normal stress whereas contact shear stresses are neglected in the assessment of the mechanical deformation. Meanwhile, the influence of contact shear stresses on the size of the contact area and therefore the normal force-displacement relationship measured in the experiments may be quite significant.

In this work we have developed an exact solution to the problem of adhesive contact of an elastic sphere with a rigid substrate. We have preserved the influence of the shear stresses on the normal displacement in the contact zone and have not applied any additional physical simplification to the solution. Using a carefully chosen general solution in the form of Papkovich-Neuber functions, a special curvilinear coordinate system, namely toroidal coordinates, and the Meler-Fok integral transform we have derived an exact analytical solution to the formulated contact problem. A detailed analysis of the contact stresses, strain, displacement, and contact zone sizes has been performed.

IC/CTS4625/09: Waves, vibrations, cracks, shocks.

Organiser: Bernard Rousselet (Université de Nice Sophia Antipolis, France)
Co-organiser: Leszek Malag (Koszalin University of Technology, Poland)

The hybrid methodology to determinate state of material during tensile test. **Leszek Malag** (Koszalin University of Technology, Poland), Leon Kukielka (Koszalin University of Technology, Poland) IC/CT3104/094

The basic problems occur the engineering calculations with finite elements method (FEM) is to acceptance the suitable form of mathematical model, which describe the mechanical properties of analyzed materials as well as obtaining the constants in this model. The macroscopic material models are published in the literature, they are elaborate on the basic tensile test and compression test, which are basic tests permitting of occur the plasticity and the ultimate strength properties. To indeed the influence factor on value of stresses and strains is the shape and dimension of specimen.
The tensile test described in the ISO norm with the foundation is test, where the ultimate strength properties in the studied specimens is average value. Using these properties in numerical calculations it causes that the essential differences between results calculations and experimental measurements occurrence of qualitative and quantitative.
In this paper is propose the new methodology to defining the stresses and strains states, where the finite elements method were used. The proposed hybrid methodology to defining the states of stresses and strains in metallic specimens, were applied in one-axial tensile test. These states were evaluated with elaborated applications in program ANSYS LS-DYNA. The present application allow to obtain the stresses and strains distributions in each place of specimen and in each time duration of the tensile test process.

Ray method for solving boundary-value dynamic problems of arbitrary spatially curved rods. **Yuriy Rossikhin** (Voronezh State University, Russian Federation), Marina Shitikova (Voronezh State University, Russian Federation) IC/CT604/094

The ray method is developed for solving boundary-value dynamic problems connected with the propagation of planes of strong and weak discontinuity in spatially curved linear elastic rods of arbitrary cross-section. Equations of three-dimensional theory of elasticity are used, which at first should be written on the wave surface with the help of the theory of discontinuities in the rectangular system of coordinates, one of which is tangential to the rod's centerline and the other two are the

main central axes of the rod's cross-section, and then are integrated over the rod's cross-sectional area. It is assumed that the discontinuities in stresses on the sections with the normals perpendicular to the rod's centerline can be neglected as compared to those on the sections with the normals parallel to the centerline. Rod's cross-sections remain to be planar during its deformation. These assumptions result in the generation of two wave surfaces in the space-curved rod which propagate with the velocities of bending-longitudinal and rotational-shear waves which are equal to $\sqrt{\frac{E}{\rho}}$ and $\sqrt{\frac{\mu}{\rho}}$, respectively, where E and μ are the longitudinal and shear moduli, respectively, and ρ is the density. When solving boundary-value problems, the values to be found are represented in terms of the ray series [1], wherein coefficients are the discontinuities in partial-time derivatives of the desired functions, and the time passed after wave front arrival at an arbitrary point is the independent variable. The ray series coefficients are determined from the recurrent equations of the ray method within an accuracy of arbitrary functions, which are found then from the boundary conditions. Similar approach was applied in [2] for investigating transient waves in thin elastic plates and shells. Examples illustrating the effectiveness of the ray method during the solution of the problems of the shock interaction, resulting in propagation of transient waves of strong discontinuity in spatially curved rods are presented. This research is supported by the Russian Foundation for Basic Research under Grant No.05-08-17936.

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Orthogonality of 3D time-harmonic modes in viscoelastic laminates and the method of far-field evaluation for finite acoustic sources. **Dmitry Zakharov** (Moscow State Univ. of Railway Engineering, Russian Federation) IC/CT864/094

Modes of an infinite laminate subjected to homogeneous boundary conditions on the faces are considered. For the general mode representation supporting angular symmetry the orthogonality relations are derived and expressed using the reciprocity theorem. Exact solutions of some particular boundary value problems are obtained. A method for exact calculation of the far field to an acoustic source given in the form of surface load or body force, localized in a finite region, is suggested. Some examples of practical interests are presented in context of modelling fields, radiated by ultrasonic transducers into the inspection solids.

Trapped modes in elastic waveguides. **Julia Postnova** (Imperial College London, UK), Richard Craster (Imperial College London, UK) IC/CT2434/094

Trapping of energy is a common feature of many wavebearing structures, here we will consider waveguides with slowly varying localized curvature or thickness. Trapped modes occur at particular frequencies (resonant frequencies) and are localized in an area of geometry variation. Localization of energy is often undesirable and it is important to avoid excitation of a structure at resonant frequencies. During the last few decades the existence of trapped modes in non-uniform acoustic and quantum waveguides has been extensively investigated. The purpose of this talk is to discuss the possibility of trapped modes in non-uniform elastic waveguides that have a perturbation in thickness or in curvature and to provide an appropriate theory for obtaining frequencies at which trapped modes are excited. We develop an asymptotic procedure which reduces the governing equations to a single ordinary differential equation including all the essential physics. It is shown that this reduced model has the same functional form for both guides (bent and topographically varying plates), therefore the two problems are mathematically identical. We consider waveguides subject to different types of boundary conditions (traction-free boundaries, rigid-clamped boundaries and a combination of them). For an acoustic bent plate with mixed boundary conditions the sign of the curvature function plays an important role in existence of trapping. We also consider the three-dimensional geometry of a topographically varying plate with waves propagating along the third dimension and decaying with a distance from it. A mathematical explanation and physical argument of the existence of trapped modes depending on different situations are given. Numerical results based upon the Newton-Kantorovich method are compared with the asymptotic solution and good agreement between two methods is shown.

Nonlinear vibrations for non-destructive testings, EDO models. **Bernard Rousselet** (Université de Nice Sophia Antipolis, France) IC/CT3430/094

Non linear vibrations for non destructive testings, ODE models

Recent experimental work show that it is possible to detect damages in structures by measuring non linear vibrations. The starting point lies in several publications of the russian school of physics (Sutin-Donskoy, 1998 Ekimov-Didenkulov-Kasakov in 1999, Zaitsev-Sas 1999); more recently Moussatov-Castagnede-Gusev(2002) .

This presentation focusses on the analysis of the response in the frequency domain of a vibrating structure submited to a force acting exactly at one or two frequencis: apparition of subharmonics, intermodulations between a high and low frequency.

Recently, G. Vanderborck has performed experiments with cables of bridges and has been able to detect defects by looking at the response in the frequency domain: intermodulations appear for the damaged cable.

Models of damage for monitoring cables and beams will be discussed here.

This type of approach has been presented in previous conferences by Vanderborck and the author (Colloque national de Calcul de structures, 2005,2007, SAVIAC 2005, and in meetings of french GDR 2501 ("Etude de la propagation ultrasonore en vue du controle non destructif")) .

IC/CTS4621/09: **Advanced modelling.**

Organiser: Yuriy Tokovyy (National Taiwan University)

Stability of viscoelastic systems under stochastic parametric excitation. **Vadim Potapov** (Dept. of Structural Mechanics, Moscow State Univ., Russian Federation) IC/CT526/096

The stability of viscoelastic systems, excited by parametric loads in the form of random Gaussian stationary processes with rational spectral densities, is investigated. Almost sure stability and stability with respect to statistical moments of different order is analyzed. The estimation of the stability is carried out with help of top Liapunov exponents. For the simulation of input random processes and for the solution of integro-differential equations a numerical method is offered. It is shown that positions of stability boundaries in considered cases differs principally from similar positions, if random loads have the form of Gaussian white noises.

Analytical determination of residual stresses in a butt weld of two thin rectangular plates. **Yuriy Tokovyy** (National Taiwan University), Chien-Ching Ma (National Taiwan University) IC/CT1096/096

Residual strains and stresses caused by welding, influence essential accuracy of manufacturing, durability, and other operational characteristics of welded members of structures. Computational-experimental methods are widely used for determination of residual stress-strain state. One of such methods is the method of conditional plastic strains which is based on the solving inverse problems of mechanics of deformable solids with eigen-strains under experimental information obtained by physical methods. Thus it is supposed that a material of the welded element of structure is elastic with exception of the weld zone which exhibits elastic-plastic behavior.

For solving above mentioned inverse problems, it is necessary for researcher to have a 'convenient' analytical solutions of corresponding direct problems, especially in the case of bounded bodies.

This report presents a technique of finding an exact analytical solution of a direct problem of determination of residual stresses in a rectangular plate with rectilinear butt weld. By solving this problem it is assumed, that two butt-welded plates make one rectangular (main) plate, and the welded seam is modeled as a field of residual strains locally distributed in the main plate. The edges of the main plate are free from force loadings. For construction of the solution to the direct problem, which consists in determination of stress state of the main plate under known field of residual strains, the analytical technique based upon direct integration of the equilibrium and compatibility equations in terms of stresses, proposed by Vihak, is used. Stress tensor components are found in the closed form of an explicit functional dependence on the given residual strains. It is proved that the stresses found are self-equilibrated.

The analysis of a residual stress state of rectangular plate for different ratio of length of its sides is carried out. Influence on a stress state of change of distribution character of residual strains in sites of welds near boundaries is investigated. Comparison of calculated results obtained by the proposed method with results of the known approximate methods is carried out, and also limits of application of the last ones are established.

Asymptotic behaviour of rigid plastic solutions in the vicinity of fictional interfaces and non-local fracture criteria. **Elena Lyamina** (Institute for Problems in Mechanics RAS, Russian Federation) IC/CT473/096

In the case of a rigid/perfectly plastic material model with arbitrary isotropic smooth yield criterion, the velocity fields adjacent to surfaces of maximum friction (surfaces where the friction stress is equal to the shear yield stress) must be describable by nondifferentiable functions where the maximum shear strain rate and the effective strain rate approach infinity. In particular, the equivalent strain rate follows an inverse square root law near the friction surfaces. Modifications of the material model may or may not change the singular character of the solutions in the vicinity of such surfaces. In particular, several models of pressure-dependent plasticity require singular velocity fields in the vicinity of maximum friction surfaces but the asymptotic behaviour of these fields depends on the specific model. A conceptual difficulty related to singular velocity fields appears if the model in question includes an evolution equation. Usually, in such cases solutions have no physical sense. The situation is very similar to that in linear elastic fracture mechanics where stresses are infinite at crack tips. A possible way to resolve this difficulty is to introduce non-local quantities. In the present paper, the initial/boundary value problem consisting of a planar deformation comprising the simultaneous shearing and expansion/contraction of a hollow cylindrical specimen of material is considered. This combined deformation ensures that there are no rigid regions, i.e. the material is everywhere in a state of yield. Symmetry in the circumferential direction dictates that all quantities are a function of the radial direction only. Such a statement of the problem permits rather a simple solution with no simplified assumptions. The material model includes a popular damage evolution equation. It is shown that the local damage parameter cannot be used because the solution has no physical sense. A non-local parameter is proposed to overcome this difficulty.

Conditional Lagrange derivative and its application in modeling of solids. **Peter Béda** (Budapest University of Technology and Economics, Hungary), Gyula Béda (Budapest University of Technology and Economics, Hungary) IC/CT2193/096

Constitutive equations play an essential role in most problems of the mechanics of continua. Such equations are used to take into account the physical properties of materials. There are numerous ways to derive constitutive equations, but no generally accepted one exists. The most critical situation can be found, when inelastic deformations are present. Our paper aims to show what to do in material modeling for an inelastic body. The method we use is based on the virtual work and on the variation of some function W with respect to the strain tensor

$$\int_{t_0}^{t_1}\int_V \sigma\cdot\cdot\delta\varepsilon dV dt \equiv \delta\int_{t_0}^{t_1}\int_V W dV dt.$$

Here, stress, strain and the variation of strain are denoted by σ, ε and $\delta\varepsilon$, respectively. The strain tensor is the Lagrange derivative $\$_\varepsilon$ of W with respect to ε, thus in the uniaxial case the constitutive equation is

$$\sigma\,(=\$_\varepsilon(W)) = \frac{\partial W}{\partial\varepsilon} - \frac{d}{dt}\left(\frac{\partial W}{\partial\dot\varepsilon}\right) - \frac{d}{dx}\left(\frac{\partial W}{\partial\varepsilon'}\right).$$

Generally, Lagrange derivative defines an elastic body. In the following we assume that an additonal equation $K=0$ should also be satisfied and calculate the Lagrange derivative of $F=W+\lambda K$. The first variation of F is called the conditional Lagrange derivative of function W. Then the possible constitutive equation reads

$$\sigma = \frac{\partial A}{\partial\varepsilon}+\lambda\frac{\partial K}{\partial\varepsilon}-\left(\frac{\partial D}{\partial\varepsilon}-\frac{\partial B}{\partial\sigma}+\lambda\frac{\partial^2 K}{\partial\dot\varepsilon\partial\sigma}\right)\dot\sigma-\lambda\frac{\partial^2 K}{\partial\dot\varepsilon\partial\varepsilon}\dot\varepsilon-\left(\frac{\partial E}{\partial\varepsilon}-\frac{\partial C}{\partial\sigma}\right)\sigma',$$

which may describe inelastic behavior, too. The conditions for λ are formulated by the material stability assumption, as in several cases. Here we use Lyapunov stability based concepts.

Modeling, analysis and simulation of the human femur: prosthesis of femur head. **Orlando Martín Hernández Bracamonte** (Universidad Nacional de Trujillo, Peru), José Manuel Olivencia Quiñones (Universidad Nacional de Trujillo, Peru) IC/CT872/009

We report the results obtained when carrying out the analysis of the strengths and strains that take place when prosthesis of femur head are implanted in the human femur. The modeling is made with tools provided by Computer Aided Geometry Design, using Non Uniform Rational B-Splines representations (NURBS). In the analysis of the strengths and strains, produced in the bone-cement-prosthesis interaction, partial differential equations of the coupled system are obtained for the displacements and deformations, that allow to analyze cases of physical and biological loads, under which will be work the implants during their useful life, which also is estimated; because of the frequent phenomenon of bony absorption and the consequent relaxation and loss of the replacement surgery. The obtained equations are solved by finite element method, with the corresponding estimation of the obtained errors. The simulations will be performed using high level software able to show realistic visualizations of the observed phenomena in real time. The fracture of the femur neck is a frequently observed trauma and has taken to the authors to make the present work. The obtained results will allow to make the modeling, analysis and simulation of other bony structures and the implants of the corresponding prosthesis.

Heuristic search for a predictive strain-energy function in nonlinear elasticity. **Dmitri Miroshnychenko** (University of Leicester, UK) IC/CT4003/092

In this work, we present a semi-structural and semi-phenomenological model (Miroshnychenko *et al.* J. Mech. Phys. Solids 53 (2005) 748–770) that emerged in a search for a more powerful and predictive strain-energy function in order to better account for nonlinear elastic behaviour of polymeric materials. This development had been led to by evaluation and comparison of predictive capability for three models: the eight-chain model (Arruda and Boyce J. Mech. Phys. Solids 41 (1993) 389–412), the first stretch invariant model, and the first and second stretch-invariant additive model to reproduce the mechanical behaviour of elastomeric materials in experiments using data due to Treloar (Trans. Faraday Soc. 40 (1944) 59–70).

The eight-chain model produces very similar results to those of the first stretch invariant model. Thus, it is shown that the former can not be greatly enhanced within the limitation of the latter or also, as it happens, of the first and second stretch-invariant additive model. However, significant improvement is critically needed in order to better cope with prediction of data due to Treloar (1944), especially in equibiaxial extension. The semi-structural and semi-phenomenological model that we propose retains the traits and corrects the faults of the eight-chain model, thus conforming more closely to the quintessential, classical data due to Treloar (1944). This composite model and its modification (the filament model) also suggest how a new structural model can be developed that would have only two material parameters and be able to outperfom previous models.

09: Solid Mechanics, Posters

IC/PP3589/092: Analysis of thermal stresses in a visco-elastic tri-material under a point heat-source.

Presenter: Ching-Kong Chao (National Taiwan University)

A general solution for a thermoviscoelastic trimaterial combined with a point heat source and a point heat sink is presented in this work. Based on the method of analytic continuation associated with the alternation technique, the solutions to the heat conduction and thermoelastic problems for three dissimilar, sandwiched media are derived. A rapidly convergent series solution for both the temperature and stress field, expressed in terms of an explicit general term of the corresponding homogeneous potential, is obtained in an elegant form. The hereditary integral in conjunction with the Kelvin-Maxwell model is applied to simulate the thermoviscoelastic properties, while a thermorheologically simple material is considered. Based on the correspondence principle, the Laplace transformed thermoviscoelastic solution is directly determined from the corresponding thermoelastic one. The real time solution can then be solved numerically by taking the inverse Laplace transform. A typical example concerning the interfacial stresses generated from a combined arrangement of a heat source and sink are discussed in detail. The corresponding thin film problem is also discussed.

Keywords: thermoviscoelasticity; trimaterial; interfacial stresses; analytic continuation

IC/PP841/094: Elastoplastic problem for cylindrical shells with crossing cracks.

Presenter: Iryna Kostenko (Lviv, Ukraine)

The solution of problem of fracture for a cylindrical shell weakened by cracks with plastical areas is constructed with using the δ_k- model. The generalized δ_k- model is used to construct a mathematical model of shell, plasticity strips at the crack extension are modelled by fictitious cracks, the faces of which are under unknown normal $N$and bending moments M. These stresses and moments satisfy the corresponding plasticity conditions for shells

The crack faces do not come in contact in the process of strain. It is assumed that the crack sizes, the load value and material behaviour are such that plastical strains develop at the crack extension in the form of a thin strip throughout the shell thickness.

Centers of cracks are allocated along the guiding $\beta = 0$ (β is normalized to radius R of a middle surface of the shell coordinate along the generatrix.) It is assumed that the shell is under the conditions of cyclic symmetry and may be considered as a cylindrical panel $|\beta| \le \beta_0$ with a crack $|\alpha| \le \alpha_0, \beta = 0$ ($\alpha_= l/R, l$ is a half-length of a real crack, $\alpha_0 = l_0/R, l_0 = l_0/R, l_0-$ length of plastical area before the top of crack, α normalized to Rcoordinate along the guiding $\beta = 0, k-$ is the number of cracks).

Numerical analysis behavior of parameter $\alpha_0 = l_0/R$, when value of parameter $N_2^0/(2h\sigma_T))$ is known. Parameter $\delta_k$is obtained from such equation:

$$\delta_k = a_1 v_1 + a_N v_N + a_M v_M,$$

where a_1, a_N, a_M- known coefficients, which was founded as a solution of system of singular integral equation satisfying the corresponding plasticity conditions for shell.

IC/PP4042/094: Longitudinal waves at a micropolar fluid/solid interface.

Presenter: Dilbag Singh (Punjab University, Chandigarh, India)
Co-author: Sushil Kumar Tomar (Panjab University, Chandigarh, India)

In this paper, we have explored the possibility of propagation of plane waves in a micropolar fluid of infinite extent. The phenomena of reflection and transmission of longitudinal elastic at a plane interface between a homogeneous micropolar fluid half-space and a micropolar solid half-space has also been investigated. It is found that there exist four plane waves propagating with distinct speeds in a micropolar fluid. All the four waves are found to be dispersive and attenuated. The reflection and transmission coefficients are found be the functions of the angle of incidence, elastic properties of the half-spaces and frequency of the incident wave. Frequency equation for the Stoneley waves at micropolar solid/fluid interface has also been derived. Numerical computations have been performed for a specific model. The dispersion curves and attenuations of existed waves in micropolar fluid have been computed and depicted graphically. The variations of various reflection and transmition coefficients are are also shown against the angle of incidence. The real and imaginary parts of phase velocity of Stoneley waves have also been plotted with non-dimensional wavenumber. Results of some earlier workers have been deduced from the present formulation.

IC/PP4890/095: Particle dynamic method for solution of physical and geometrical nonlinear problems of elasticity.

Presenter: Muaed Oshkhunov (Kabardino-Balkarian State University, Russian Federation)

The discrete method of solid media into interactions particles is presented. Interaction potential between particles depends only on distance and may imitate physical and geometrical nonlinear properties of media. Classic problems of elasticity are realized as limit state with respect to time of dynamic system of particles. Various discrete models and relations of these algorithms with finite element methods are discussed. The numerical results and comparison with the classic solutions of elasticity are presented. Besides the temperature and phase confirmation are also considered.

IC/PP912/096: Variational coupled formulation of the Navier–Stokes problem in Lagrangian coordinates.

Presenter: Natalia Tuchkova (Russian Academy of Sciences, Moscow)
Co-author: Sergey Lurie (Russian Academy of Sciences, Moscow)

The variational formalism of formulation of non-holonomic media models is offered. This approach is based on the formal generalization of continued mechanics models of deformable bodies on the four-dimensional space of events with a four-dimensional vector of the generalized displacements. Time of process is included in the generalized four-dimensional system of coordinates and considered as one of independent coordinates.

As kinematic connections it is proposed to use generalized the Cauchy relations for a four-dimensional vector of the generalized displacement media: a four-dimensional vector of the generalized displacement. The general form of the constitutive equations for non-holonomic media is established. These constitutive equations are defined with the help of the non-integrability conditions for possible work of internal force factors.

The variational equation non-holonomic linear media is obtained and the appropriate initial and boundary problems are formulated. It is proved strictly, that within the framework of the offered model irreversible processes proceed with positive dissipation, and the second law of thermodynamics takes place. In result, the couple model of the dynamic thermoelasticity with dissipative properties is formulated and the appropriate initial -boundary problems is written. As a special case the combined model of creep and a relaxation is received.

The couple variational formulation of the Navier–Stokes problem in Lagrangian coordinates is obtain, allowing to formulate the consistent system of initial and boundary conditions. Within the framework of specific model the generalized equation of heat conductivity is received, the treatments of Fourier hypothesis (for heat flow) and Duamel–Neumann hypothesis are given also.

This work is supported by the Russian Foundation for Basic Research (Project 05-07-90134 and Project 06-01-00051).

[1] Gorshkov A., Lurie S.; Mechanics of Solids. Transl. Allerton Press as Mekhanika tverdogo tela (2006), 6.

IC/PP4187/096: Stochastic finite-layer method.

Presenter: Marek Wyjadlowski (Technical University Wroclaw, Poland)

The finite layer method provides the efficient method for the analysis of soil deposits which are horizontally stratified. The method can be used to analyse the settlement under two and three dimensional conditions. The settlement of horizontally layered soil deposits can be analysed by breaking the load into Fourier Components. For better accuracy, a larger number of harmonics is required for computations. Each of these Fourier components can be analysed separately and the final solution can be obtained by syntetizing the component solutions. The paper deals with the analysis of randomly inhomogeneous media as soils. In many practical cases, the soil profile can be approximated by horizontal layers which have properties varying in the horizontal directions. The paper combines the FLM and effective Stochastic techniques Monte Carlo Simulation to solve the problem of foundation settlement.

IC/PP762/015: Deformation state of flexible cylindrical shells in pre-critical region.

Presenter: Olga Tumashova (Lvivska Politechnica, Ukraine)

The problems of equilibrium of thin elastic shells in precritical region of deforming are given with the nonlinear systems of connectied differential equations. The problems of deforming thin elastic cylindrical shells with variable thickness and curvature in one direction, based on the solving two-dimentional nonlinear problem. This nonlinear problem are solved using difference approximations, linearization, a stable method of discrete orthogonalization. Consider the elastic shallow cylindrical panel $(2a * 2b)$ with variable thichness and curvature, which is under the normal surface load q. Describing nonlinear task about the strain of shallow shells under the strength influences in supposition, that curvature or thickness-variables can be written down, as the solving system of differential equa-

tions of type:

$$\begin{aligned} \frac{\partial \vec{N}}{\partial x} &= \vec{F}(x, y, \vec{N}, \frac{\partial \vec{N}}{\partial y}, \frac{\partial^2 \vec{N}}{\partial y^2}, \frac{\partial^3 \vec{N}}{\partial y^3}, \frac{\partial^4 \vec{N}}{\partial y^4}, q) \\ B_1 \vec{N} &= \vec{b}_1\,, \quad x = \pm a \\ B_2 \vec{N} &= \vec{b}_2\,, \quad y = \pm b \quad , \end{aligned}$$

where $\vec{N} = \{N_x, N_{xy}, Q_x, M_x, u, v, w, \vartheta_x\}$.

This nonlinear problem is solved using the methods: difference approximations, linearization and discrete orthogonalization. Consided the deformation of the elastic shallow cylindrical panel with variable thickness and curvature is under the influence of normal surface load q.

10: Fluid Mechanics, Minisymposia

IC/MP290/010: **Multiphysics and multiscale methods in hydrodynamics.**

Organiser: Luca Bonaventura (Politecnico di Milano, Italy)
Co-organiser: Fausto Saleri (Politecnico di Milano, Italy)
Co-organiser: Edie Miglio (Politecnico di Milano, Italy)

The simulation of complex hydrodynamics phenomena involves the presence of different space and time scales and different physical phenomena. In order to resolve all the time and space scales a full 3D Navier–Stokes system should be solved; in practice this is too expensive from the computational point of view hence the use of some reduced (low-dimensional or simplified) models is advisible. The adoption of these simplified models in all the domain can cause a low level of accuracy in the solution so a suitable coupling between the full model and the reduced ones is required. The same idea can be used in order to (partially) include 3D effects into 2D models (or 2D effects into 1D models). Moreover, even from the physical point of view, some effects due to complex phenomena occuring in water flow (e.g. sedimentation) can be simulated by means of suitable reduced model.

The aim of the minisymposium is to collect contributions emphasizing the usefulness of multiscale and multiphysics methods in order to efficiently solve the above mentioned problems.

An iterative procedure to solve a coupled athmosphere-ocean turbulence model. **Tomás Chacón Rebollo** (Universidad de Sevilla, Spain), Stephane Del Pino (Commissariat à l'Energie atomique, France), Driss Yakoubi (Université Pierre et Marie Curie, France) IC/MT1568/010

In this contribution we focus our attention on the modelling of the surface layer between the athmosphere and the ocean. We are interested in designing effective procedures to solve the following coupled model:

$$\begin{aligned} -\nabla\cdot(\alpha_i(k_i)\nabla\mathbf{u}_i)+\nabla p_i &= \mathbf{f}_i && \text{in } \Omega_i,\\ \nabla\cdot\mathbf{u}_i &= 0 && \text{in } \Omega_i,\\ -\nabla\cdot(\gamma_i(k_i)\nabla k_i) &= \alpha_i(k_i)|\nabla\mathbf{u}_i|^2 && \text{in } \Omega_i,\\ \mathbf{u}_i &= 0 && \text{on } \Gamma_i,\\ k_i &= 0 && \text{on } \Gamma_i,\\ \alpha_i(k_i)\partial_{\mathbf{n}_i}\mathbf{u}_i - p_i\mathbf{n}_i + c_i(\mathbf{u}_i-\mathbf{u}_j)|\mathbf{u}_i-\mathbf{u}_j| &= 0 && \text{on } \Gamma,\\ k_i &= \lambda|\mathbf{u}_1-\mathbf{u}_2|^2 && \text{on } \Gamma, \end{aligned} \tag{1}$$

where Ω_i is a bounded domain of $\mathbb{R}^d$, of boundary $\partial\Omega_i = \Gamma_i \cup \Gamma$, $\Gamma = \partial\Omega_1 \cap \partial\Omega_2$ being the interface between the two fluids. Γ is assumed to be flat. Each of the two turbulent fluids is modelled by a simplified one-equation turbulence model whose unknowns are the velocity $\mathbf{u}_i$ and the turbulent kinetic energy (TKE) k_i. In the first equation we model the generation of eddy viscosity. The quantity $\alpha_i(k_i)$ is the turbulent viscosity. The fluids are assumed to be incompressible (second equation). In the third equation we model the generation of TKE by means of a production source term, and also the turbulent dissipation of TKE: the function $\gamma_i(k_i)$ is also a turbulent diffusion. We assume non-slipping boundary conditions in the boundary parts Γ_i for simplicity (fourth and fifth equations). The sixth equation globally models the interaction of the two boundary layers on one and another side of the interface Γ as friction effects, by means of a set of boundary conditions similar to Manning's law. Finally, the last equation models the generation of TKE in the interface. The coefficients c_i and λ are positive. We assume that the turbulent diffusions α_i, γ_i belong to $W^{1,\infty}(\mathbb{R})$ and verify that $\alpha_i \geq \nu$ and $\gamma \geq \nu$, for some $\nu > 0$. The eddy diffusions usually are unbounded functions, but this renders the analysis extremely hard, so we consider a simplified model, that still includes several realistic non-linear interactions.

This system was studied[1] where existence and uniqueness of small smooth solutions were proved. Spectral and Finite Element discretizations were studied in subsequent papers by the same authors and co-workers. In these papers, the ability of these discretization techniques to approach the solutions of model (1) was proved. However, in both cases the discretizations achieved consisted in fully non-linear sets of algebraic equations.

Our purpose here is to derive iterative procedures to solve our system that decouple the interactions of the problem, leading mainly to linear problems.

Iterative procedure. Let us introduce the function space $\mathbf{X}_i = \{\mathbf{v} \in \mathbf{H}^1(\Omega_i)^d;\ \mathbf{v} = 0 \text{ on } \Gamma_i\}$. Consider also two conjugate positive real numbers r and r' such that $r > d$. We introduce the following iterative procedure to solve the coupled system:

find $(\mathbf{u}_i^{n+1}, p_i^{n+1}, k_i^{n+1}) \in \mathbf{X}_i \times L^2(\Omega_i) \times W^{1,r'}(\Omega_i)$, such that $\forall \mathbf{v}_i \in \mathbf{X}_i$:

$$(\alpha_i(k_i^n)\nabla\mathbf{u}_i^{n+1}, \nabla\mathbf{v}_i)_{\Omega_i} - (\nabla\cdot\mathbf{v}_i, p_i^{n+1}) + c_i(|\mathbf{u}_i^{n+1}-\mathbf{u}_j^{n+1}|(\mathbf{u}_i^{n+1}-\mathbf{u}_j^{n+1}), \mathbf{v}_i)_\Gamma = (\mathbf{f}_i, \mathbf{v}$$

and $\forall q_i \in L^2(\Omega_i)$ we require that $(\nabla\cdot u_i^{n+1}, q_i) = 0$, with $k_i^{n+1} = 0$ on Γ_i, $k_i^{n+1} = \lambda|\mathbf{u}_1^{n+1} - \mathbf{u}_2^{n+1}|^2$ on Γ, such that

$$\forall \phi_i \in W_0^{1,r}(\Omega_i),\ (\gamma_i(k_i^n)\nabla k_i^{n+1}, \nabla\phi_i)_{\Omega_i} = (\alpha_i(k_i^n)|\nabla\mathbf{u}_i^{n+1}|^2, \phi_i)_{\Omega_i}. \tag{2}$$

Observe that the problem for the $\mathbf{u}_i^{n+1}$ (first equation in (.1)) is in reality non-linear due to the presence of the Manning-like source term. This is a mild non-linearity due to the monotonic nature of this term, that may be made explicit in practice if mass-lumping techniques are used.

Our main result states that if the sequences $(\mathbf{u}_i^n)_n$ and (k_i^n) are bounded in $W^{1,3+\epsilon}(\Omega_i)^d$ and $W^{1,3}(\Omega_i)$, then, for small enough data (in a convenient sense), the iterative scheme (.1)–(2) is contracting. This proves in addition the uniqueness of solutions of the coupled model.

We shall present some numerical tests realized with the software FreeFEM3D (see [2]) in meaningful situations, that agree with the expectations of this result.

[1] Bernardi,C., Chacon Rebollo, T., Lewandowski, R. and Murat, F.; A model for two coupled turbulent fluids. Part I: Analysis of the system. In Nonlinear partial differential equations and their applications. Collège de France Seminar, Vol. XIV (Paris, 1997/1998), 69–102, Stud. Math. Appl., 31, North-Holland, Amsterdam, 2002.

[2] Del Pino, S. and Pironneau, O.; http://www.freefem.org/ff3d.

Assimilation of images for river hydraulic simulations. **Jérôme Monnier** (Université Grenoble I, France), Xijun Lai (Chinese Academy of Sciences), Marc Honnorat (Université Grenoble I, France), Francois-Xavier Ledimet (INRIA Rhône-Alpes, France) IC/MT2664/010

A major difficulty in the numerical simulation of river hydraulic flows is bound to model parameters definition. Variational data assimilation makes it possible to combine the model and observation data in order to identify the value of model parameters consistent with reality. However, in river hydraulics, observation data are available only in very small quantities. Water level measurements can be available at gauging stations, but it is the main channel only and they are very sparse in space. Velocity measurements are even rarer and uncertain, since they require complex human interventions. Consequently, in practice these observations are usually not sufficient to take full advantage of data assimilation for identification purposes. This lack of data is all the more problematic in case of extreme events such as floods. Thus, remote sensing data such as video and spatial images offer a large potential which is not fully exploited yet. In this talk, we address the assimilation (in

addition to classical data)of the following two types of images : 1) video images of particles flowing at surface; 2) satellite images of the flood plain. In case 1), this led us to extend the method to extra lagrangian data. The trajectory of particles advected by the flow bring information on the surface velocity using an extra transport model. In case 2), we defined an appropriate cost function and adopted a temporal strategy into the variational data assimilation process. These methods are implemented into our software DassFlow. The direct code is a HLLC Riemann solver for 2D shallow-water equations. The cost functions are minimized using a Quasi-Newton algorithm, which implies the computation of its gradient using an adjoint model. The latter is created with the help of the automatic differentiation tool Tapenade. Numerical twin data assimilation experiments demonstrate that these approaches makes it possible to improve the identification of model parameters. If considering real flows, difficulties arising from the shallow-water model incompleteness are pointed out. **References** 1. "Lagrangian data assimilation for river hydraulics simulations" M. Honnorat, J. Monnier, FX Ledimet. Submitted. 2. "Assimilating spatial distributed water level into hydraulic models" X. Lai, J. Monnier. Submitted.

Adaption of hierarchical multiscale hydrodynamical models. **Daniela Capatina-Papaghiuc** (Université de Pau et des Pays de l'Adour, France), Mohamed Amara (Université de Pau et des Pays de l'Adour, France), David Trujillo (Université de Pau et des Pays de l'Adour, France) IC/MT1912/010

We are interested in the hydrodynamical modeling and numerical simulation of an estuarian river flow. Since the use of a realistic 3D model would engender a huge computational cost, our goal is to implement different lower-dimensional models on adequated regions of the river and then to automatically couple them. Several 2D and 1D hydrodynamical models of shallow water type exist in the literature, but their mathematical justification is rather heuristic. We employ here some new hydrodynamical models, derived in a unified manner in a variational framework. For this purpose, we put the physical time-discretized 3D problem, based on the Navier-Stokes equations and satisfying natural boundary conditions, under a nonlinear mixed weak form and then we obtain the simpler models by a projection method. This approach avoids any closure problem that one usually encounters in the shallow water system and moreover, all the models provide a 3D velocity and pressure.

The key point is that we thus get hierarchical models : the 1D problem is a conforming approximation of the 2D horizontal, respectively vertical models, which are both conforming approximations of the 3D one. This hierarchy allows a natural coupling, in the sense that the transmission conditions between the different models are implicitly contained in the formulations. The coupling is then achieved through residual *a posteriori* error indicators. One can note that a different coupling strategy, also based on *a posteriori* model estimators using the dual-weighted residual method, was developed by Braack and Ern and applied to the shallow water system by Perotto.

In this talk, we briefly describe the derived models, their mathematical analysis and the comparison with the classical shallow water equations and then we focus on the model adaption. We define the model indicator between the 3D model and a generic lower-dimensional approximation and we prove its reliability. For this purpose, we adapt a result of Brezzi, Rappaz and Raviart established for finite dimensional approximations of nonlinear problems to our multiscale approximation at the continuous level. Finally, the discretization of the previous models will be discussed and numerical tests will be presented, illustrating the implementation of the adaptive coupling between the 1D and any of the two 2D models.

IC/MP290/010: Multiphysics and multiscale methods in hydrodynamics. #2

Organiser: Luca Bonaventura (Politecnico di Milano, Italy)
Co-organiser: Fausto Saleri (Politecnico di Milano, Italy)
Co-organiser: Edie Miglio (Politecnico di Milano, Italy)

(For abstract, see session #1 above.)

A section-averaged model for mobile-bed river hydraulics. **Alberto Deponti** (Università degli Studi di Torino, Italy), Luca Bonaventura (Politecnico di Milano, Italy), Edie Miglio (Politecnico di Milano, Italy), Giorgio Rosatti (Università degli Studi di Torino, Italy) IC/MT1411/010

A section-averaged model for mobile-bed river hydraulics is presented and analysed. The model is based on the conservation equations of liquid mass, solid sediment mass and momentum. By using appropriate closure formulae for sediment transport and for bottom friction, a system of three non-linear hyperbolic equations is obtained. In particular, for the sediment transport process, empirical closure formulae are used; these impose a highly non-linear relation between sediment and liquid discharges. The equations are averaged over the channel cross-section in order to account for irregular geometries. By using appropriate averaging coefficients, the model is capable to account for two-dimensional phenomena such as non–uniformities in velocity distribution and sediment transport across the section, non-uniformities in bottom friction and in morphological modification along the wet contour.

Analysis of the system eigenstructure shows the importance of considering arbitrary cross-sections for properly describing hydraulic flows and morphological modifications of the cross-section induced by sediment transport process. The analysis also shows that these two physical processes are strongly coupled throughout a wide region of flow regimes around unitary Froude number; particularly, the width of this region is strongly affected by cross-section geometry and by the sediment transport regime. For these reasons, a coupled numerical model is implemented. The model imposes the conservation of total mass (liquid and solid) and computes hydraulic flows and morphological modifications of the cross-section at the same time. Applications to idealised benchmarks and realistic test cases will be presented and discussed.

High-order upwind scheme for modelling turbulent shallow water flow in hydraulic structures. **M. Elena Vazquez-Cendon** (Universidade de Santiago de Compostela, Spain), Luis Cea (Universidade da Coruña, Spain) IC/MT2419/010

An unstructured finite volume model for quasi-2D free surface flow with wet-dry fronts and turbulence modelling is presented.

The convective flux is discretised with either a an hybrid second-order/first-order scheme, or a fully second order scheme, both of them upwind Godunov's schemes based on Roe's average. The hybrid scheme uses a second order discretisation for the two unit discharge components, whilst keeping a first order discretisation for the water depth. In such a way the numerical diffusion is much reduced, without a significant reduction on the numerical stability of the scheme, obtaining in such a way accurate and stable results. It is important to keep the numerical diffusion to a minimum level without

loss of numerical stability, specially when modelling turbulent flows, because the numerical diffusion may interfere with the real turbulent diffusion.

In order to avoid spurious oscillations of the free surface when the bathymetry is irregular, an upwind discretisation of the bed slope source term [1] with second order corrections is used. In this way a fully second order scheme which gives an exact balance between convective flux and bed slope in the hydrostatic case is obtained.

The $k-\varepsilon$ equations are solved with either an hybrid or a second order scheme [3].

The results given by a first order scheme, the hybrid scheme and the fully second order scheme are compared in several free surface shallow flows. A first order scheme may give rather good predictions for the water depth [3], but it introduces too much numerical diffusion and therefore, it excessively smooths the velocity profiles. This is specially important when comparing different turbulence models, since the numerical diffusion introduced by a first order upwind scheme may be of the same order of magnitude as the turbulent diffusion. In all the numerical simulations the importance of using a second order upwind spatial discretisation has been checked.

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A Roe-type scheme for two-phase gravitational granular flows with bottom topography. **Marica Pelanti** (École Normale Supérieure de Paris, France) IC/MT2411/010

We study a depth-averaged model of gravity-driven mixtures of solid grains and fluid flowing over non-flat basal surface. In particular, we are interested in applications to geophysical flows such as avalanches and debris flows, which typically involve both solid material and interstitial fluid.

The model system consists of mass conservation and momentum balance equations for the solid and fluid components, and it can be shown to be hyperbolic at least when the difference of phase velocities is sufficiently small.

Difficulties in the numerical approximation of the model equations arise from the presence of non-conservative products that involve the derivatives of the unknowns and that couple together the sets of equations of the two phases. Here we numerically solve the model system by a high-resolution finite volume scheme based on a Roe-type Riemann solver. Several numerical tests are presented and discussed. In particular, we show that numerical results of the two-phase model with indefinitely large interphase drag agree with the exact solution of the reduced model that can be derived theoretically by assuming that drag is strong enough to drive instantaneously phase velocities to equilibrium.

Work done in collaboration with François Bouchut (ENS Paris) and Anne Mangeney (IPGP).

IC/MP21/033: Theoretical aspects of 3D water waves.

Organiser: Gérard Iooss (Université de Nice Sophia Antipolis, France)
Co-organiser: Mark Groves (Loughborough University, UK)

The theory of two-dimensional water waves has seen a vigorous renewal of interest in the last fifteen years, a development fuelled by the emergence of powerful new mathematical methods such as spatial dynamics and variational techniques. The study of three-dimensional water waves has additional mathematical difficulties, in particular due to the presence of a two-dimensional free surface (with or without surface tension), the impossibility of using complex-variable techniques (which are well adapted to two-dimensional potential flows), and the occurence of a richer set of inherent symmetries. However, three-dimensional waves are certainly the more interesting variety from a physical point of view. The last five years have witnessed significant progress in this area, including results at a mathematical level (concerning periodic or spatially localised waves), at a numerical level (new fundamental simulations of large amplitude waves), and at an experimental level (involving experiments designed to explain observations and inspire theoreticians). This minisymposium presents an interdisciplinary spectrum of researchers working on three-dimensional water waves and focuses upon mathematical results on the Euler equations (with a free surface or interface) and studies of model equations.

On solitary water-wave interactions. **Walter Craig** (McMaster University, Canada) IC/MT3429/033

tba

Existence and stability of fully-localised 3D gravity-capillary solitary water-waves. **Mark Groves** (Loughborough University, UK) IC/MT3557/033

A solitary wave of the type advertised in the title is a critical point of the Hamiltonian, which is given in dimensionless coordinates by

$$H(\eta,\xi)=\int_{\mathbb{R}^2}\left\{\frac{1}{2}\xi G(\eta)\xi+\frac{1}{2}\eta^2+\beta\sqrt{1+\eta_x^2+\eta_z^2}-\beta\right\},$$

subject to the constraint that the impulse

$$I(\eta,\xi)=\int_{\mathbb{R}^2}\eta_x\xi$$

is fixed. Here $\eta(x,z)$ is the free-surface elevation, ξ is the trace of the velocity potential on the free surface, $G(\eta)$ is a Dirichlet-Neumann operator and $\beta>1/3$ is the Bond number.

In this talk I show that there exists a minimiser of H subject to the constraint $I=2\mu$, where $0<\mu\ll 1$. The existence of a solitary wave is thus assured, and since H and I are both conserved quantities its stability follows by a standard argument. 'Stability' must however be understood in a qualified sense due to the lack of a global well-posedness theory for three-dimensional water waves.

Non-symmetric three-dimensional gravity water waves: part I. **Gérard Iooss** (Université de Nice Sophia Antipolis, France), Pavel Plotnikov (Lavrentyev Institute of Hydrodynamics, Russian Federation) IC/MT5015/010

We consider travelling water waves in a potential flow on an infinitely deep fluid layer, which form a bi-periodic horizontal pattern on the free surface, in absence of surface tension. The pattern is not of diamond type, the two basic wave vectors K_1 and K_2 having different lengths. The waves may be considered as the nonlinear superposition of two plane waves, with corresponding wave numbers K_1 and K_2, and amplitudes ε_1 and ε_2, provided that at the bifurcation, K_1, K_2 and the bifurcation parameters μ (built with a wave length, the acceleration of gravity and the velocity of the waves) and the direction of propagation $\mathbf{u}_0$, satisfy the dispersion relation.

We first show how to build the asymptotic expansion of bifurcating 3-dimensional waves defined up to a horizontal shift, as a power series of the amplitudes $\varepsilon_1, \varepsilon_2$, the direction of propagation being close to $\mathbf{u}_0$. All coefficients may be computed explicitely in terms of the two angles made by K_1 and K_2 with $\mathbf{u}_0$. Due to the *occurence of small divisors*, the main difficulty for proving the existence of solutions, possessing the above asymptotic expansions, is the inversion of the linearized operator at a non trivial point, for applying the Nash–Moser theorem. This operator is the sum of a second order differentiation along a certain vector field (having a *non zero rotation number*), and an integro-differential operator of first order, both depending periodically of coordinates.

The idea of the method follows [1] and [2], with the additional difficulty due to the above non-zero rotation number. This talk shows *how to proceed formally* to this inversion provided two irrationality conditions on the parameters are realized. The precise conditions are provided in the next talk by P. Plotnikov.

[1] Iooss, G. and Plotnikov, P.I.; Three-dimensional doubly-periodic travelling water waves. Preprint INLN, 2006. Memoirs of AMS (to appear) (119p.).

[2] Iooss, G., Plotnikov, P.I. and Toland, J.; Standing waves on infinitely deep perfect fluid under gravity. Arch. Rat. Mach. Anal. 177 (2005),3, pp.367–478.

Non-symmetric three-dimensional gravity water waves: part II. **Pavel Plotnikov** (Lavrentyev Institute of Hydrodynamics, Russian Federation), Gérard Iooss (Université de Nice Sophia Antipolis, France) IC/MTR/

We consider periodic waves at the surface of an infinitely-deep perfect fluid, only subjected to gravity g and resulting from the nonlinear interaction of two symmetric travelling waves with the wave vectors K_1, K_2 and magnitudes ε_i. We deal with non-resonance case when the dispersion equation has the only basic symmetric solution in the lattice of periods. Our goal is to prove of existence of solutions to the nonlinear problem bifurcating from the trivial solution close to the asymptotic solutions constructed in the lecture by G. Iooss. The essential difficulty here is that we assume the absence of surface tension, which leads to a so-called *small divisor problem*. As it was shown in the previous lecture by G. Iooss that the linearised operator at a non-trivial point can be reduced, by the change of independent variables , to a canonical pseudodifferntial operator with constant coefficients in the principal part. The peculiarity of our problem is that the small divisors form clusters in the lattice of periods. We employ a modification of the Weyl theory on uniform distributions of irrational numbers modulo 1 to deduce the effective estimates of small divisors and to prove the invertibility of the principle part of the canonical operator. The most substantial ingredient of our approach is the descent method which allows to reduce the canonical pseudodifferential equation on the 2-dimensional torus to a Fredholm type equation (see[1,2]). Finally we exploit the Nash–Moser implicit function theorem and prove the existence of bifurcating doubly-periodic symmetric waves for any value of the parameters ε_i in a product of one-dimensional Cantor sets dense at 0.

[1] Iooss, G. and Plotnikov, P.I.; Three-dimensional doubly-periodic travelling water waves. Preprint INLN, 2006.

[2] Iooss, G., Plotnikov, P.I. and Toland, J.; Standing waves on infinitely deep perfect fluid under gravity. Arch. Rat. Mach. Anal. 177 (2005),3, pp.367–478.

IC/MP21/033: Theoretical aspects of 3D water waves. #2

Organiser: Gérard Iooss (Université de Nice Sophia Antipolis, France)
Co-organiser: Mark Groves (Loughborough University, UK)

(For abstract, see session #1 above.)

Gravity-capillary lumps and related problems. **Triantaphyllos Akylas** (MIT, USA) IC/MT583/033

Fully localized three-dimensional solitary waves, commonly referred to as *lumps*, have received far less attention than two-dimensional solitary waves in dispersive wave systems. Most studies have considered the long-wave limit where lumps are described by the Kadomtsev–Petviashvili (KP) equation. In the water-wave problem, in particular, lumps of the KP type are possible only in the strong-surface-tension regime, a condition that limits the water depth to a few millimetres.

We report on a new class of lumps that is possible under less restrictive physical conditions. Rather than long waves, these lumps bifurcate from linear sinusoidal waves of finite wavenumber at an extremum of the phase speed. As the group and phase velocities are equal there, small-amplitude lumps resemble fully localized wavepackets with envelope and crests moving at the same speed, and the wave envelope along with the induced mean-flow component are governed by a coupled Davey–Stewartson equation system of elliptic-elliptic type. The lump profiles feature algebraically decaying tails at infinity owing to this mean flow.

In the case of water waves, lumps of the wavepacket type are possible when both gravity and surface tension are present on water of finite or infinite depth. Moreover, a linear stability analysis of gravity-capillary solitary waves, that also bifurcate at the minimum phase speed, reveals they are unstable to transverse perturbations, suggesting a mechanism for the generation of lumps.

This generation mechanism is further explored in the context of the two-dimensional Benjamin (2-DB) equation, a generalization to two spatial dimensions of the model equation derived by T.B. Benjamin for uni-directional small-amplitude long interfacial waves in a two-fluid system with strong interfacial tension.

Dynamics of solitary gravity-capillary waves. **Paul Milewski** (University of Wisconsin, Madison, USA) IC/MT3467/033

In contrast with gravity waves, where localized, solitary waves exist only in two dimensions and only in shallow water, localized capillary–gravity waves exist in any depth and in both two and three dimensions. In three dimensions these waves were recently found, numerically, in a variety of models and in the full Euler equations ([Milewski], [Yang and Akylas], [Parau, Vanden-Broeck and Cooker]) and proven to exist analytically ([Groves and Sun]).

Little, however, is known about their dynamics. Although some aspects of these waves may be described using Nonlinear Schrödinger type equations, these equations do not seem to capture important features of the waves and their dynam-

ics. We discuss these differences and propose model equations in two and three dimensions which capture more closely the features and dynamics of the waves as compared to full Euler calculations in two-dimensions. The unidirectional model equation, in two dimensions, takes the form

$$R_t + i\mathcal{H}R = \mathcal{N}(R)\,, \tag{1}$$

where $\mathcal{N}$ is a quadratic nonlinear term and where the linear operator has the full deep-water capillary-gravity Fourier symbol

$$\widehat{\mathcal{H}} = sign(k)\sqrt{|k|(1+k^2)}\,. \tag{2}$$

We also discuss briefly the forced problem where waves are generated by a moving pressure force, simulating some aspects of wind-wave generation.

This is joint work with Benjamin Akers.

Long internal-wave models. **Jean-Claude Saut** (Université Paris-Sud, France) IC/MT3460/033

We present a systematic derivation of long waves models for internal waves together with a rigorous justification. This is a work in collaboration with Jerry Bona, Thierry Colin and David Lannes.

Justification of 3D asymptotics for water-waves. **David Lannes** (Université de Bordeaux, France) IC/MT4125/010

The water-waves equations admit many kinds of asymptotic regimes, depending on the physical characteristics of the flow: shallow/deep water, large/small amplitude, long/short waves, isotropic/anisotropic, bottom variations, etc. Such asymptotic models include: KP equation, 2DH Boussinesq, Shallow-water, Green-Naghdi, Serre equations, etc.

A systematic way to derive all the corresponding asymptotic models will be described. In order to rigorously justify them (i.e., in order to prove that their solutions converge to the exact solution of the full water-waves equations), a general well-posedness theorem for the water-waves equations will be proved. A crucial point is the boundedness of a particular energy, uniformly with respect to all the physical parameters.

IC/MP967/100: Complex flows: theoretical and computational aspects.

Organiser: Nils Svanstedt (Chalmers University of Technology, Sweden)

The minisymposium will view theoretical modeling of complex flows in porous media, in fluid/structure interaction and in heterogeneous fluids. Various tools for upscaling will be presented. The symposium will also view recent development in computational aspects of complex flows. Various multiscale finite element approaches will be presented.

Adaptive variational multiscale methods: a general framework. **Axel Målqvist** (UC San Diego, USA), Michael Holst (University of California, San Diego, USA), Mats Larson (Umeå University, Sweden) IC/MT1278/100

We present a framework for construction and error analysis of adaptive variational multiscale methods. We use a systematic technique for approximating the impact of the fine scale part of the solution on the coarse scale part of the solution. The fine scale is approximated by a sum of solutions to decoupled localized problems, which are solved numerically on a fine grid partition of a patch of coarse grid elements. The sizes of the patches of elements may be increased to control the error caused by localization. We derive error estimates in the energy norm which captures the dependency of the crucial discretization parameters: the coarse grid mesh size, the fine grid mesh size, and the sizes of the patches. Based on the error estimates we present an adaptive algorithms that automatically tunes these critical parameters.

Homogenization of gas–water flow processes in porous media. **Insa Neuweiler** (Universität Stuttgart, Germany) IC/MT2220/100

Modeling of water balances in partly saturated heterogeneous porous media often requires upscaled flow models. Such upscaled models can be derived using homogenization theory. They are based on a scale expansion and are therefore valid for specific flow regimes. Upscaled models and their effective parameters will be discussed for gravity dominated and for capillary dominated flow.

The effective parameters of the upscaled models depend on the structure of the heterogeneous parameter field. If the detailed structure is unknown, estimates have to be found, which are based on a simple characterization of the heterogeneity. Usually heterogeneous structure is characterized by second order statistical moments of the parameter fields (i.e. variance and correlation function). However, only multi-Gaussian fields are sufficiently characterized by these parameters. Stochastic properties of natural soil are mostly far from multi-Gaussian. If fields are not multi-Gaussian, other measures such as connectivity of certain materials could be better suited to characterize heterogeneous structures. The influence of connected paths of different parameter values will be demonstrated and different methods to quantify connected structures will be discussed.

Differential effective medium theory is a method to estimate the effective parameters, where information about measures for the connected structures can be taken into account. It will be demonstrated, that such methods yield better predictions than second order theory methods, if fields have connected extreme values. Except for the effective model parameters, connected parameter structures have an influence of the trapping of fluid during the flow process, which may lead to irregular fluid distributions or an unstable displacement front. The influence of trapping will also be discussed in the talk.

The work was done in collaboration with Hartmut Eichel and Hans-Jörg Vogel.

Multiscale mixed/mimetic FEM on complex geometries. **Stein Krogstad** (SINTEF ICT, Norway), Jørg Aarnes (SINTEF, Norway), Knut-Andreas Lie (SINTEF ICT, Norway) IC/MT2295/100

We consider a multiscale mixed finite element method (MsMFEM) for the modelling of porous media flow on models with complex geometrical features. The MsMFEM formulation is based on a hierarchical grid approach, where subscale effects are taken into account through the use of basis functions which are numerical solutions of local subscale/subgrid flow problems. By using these basis functions to discretize the global flow equations on a coarse grid, one can retain the efficiency of an upscaling method, while at the same time produce detailed and conservative velocity fields with subgrid resolution.

In reservoir simulation, the subgrid is typically given by a geomodel represented in a corner-point grid format, which is the industry standard for modelling complex reservoir geometry. As a result, the subgrid may be highly irregular. Thus, to apply the MsMFEM to such models, there are mainly two challenges. First, one needs a stable and conservative subgrid-solver for the local flow problems, and second, one needs means of choosing suitable coarse grids.

In this talk, we focus on the second challenge, coarse gridding for MsMFEM on models with complex geometrical features. One of the main advantages of the MsMFEM formulation is in the great flexibility with respect to grids. In fact, the coarse grid can in principle be any partition of the subgrid, where each coarse block is a connected collection of subgrid cells. However, we argue that in the process of generating coarse grids, one should follow certain simple guidelines to improve overall accuracy. Based on these guidelines, we discuss processing techniques aiming towards a fully automated gridding procedure. The presented methodology will be illustrated through numerical examples.

Stochastic homogenization of convection–diffusion problems. **Nils Svanstedt** (Chalmers University of Technology, Sweden) IC/MT2892/100

We study the asymptotic behaviour for a class of convection–diffusion problems where both the convection field and the diffusion process are random. By using G-convergence for monotone operators we obtain a homogenized problem where the homogenized operator is chaeacterized explicitly. Wee also show some numerical simulations.

IC/MP3867/101: Experimental and numerical aspects of 3D water waves.

Organiser: Gérard Iooss (Université de Nice Sophia Antipolis, France)
Co-organiser: Mark Groves (Loughborough University, UK)

The theory of two-dimensional water waves has seen a vigorous renewal of interest in the last fifteen years, a development fuelled by the emergence of powerful new mathematical methods such as spatial dynamics and variational techniques. The study of three-dimensional water waves has additional mathematical difficulties, in particular due to the presence of a two-dimensional free surface (with or without surface tension), the impossibility of using complex-variable techniques (which are well adapted to two-dimensional potential flows), and the occurence of a richer set of inherent symmetries. However, three-dimensional waves are certainly the more interesting variety from a physical point of view. The last five years have witnessed significant progress in this area, including results at a mathematical level (concerning periodic or spatially localised waves), at a numerical level (new fundamental simulations of large amplitude waves), and at an experimental level (involving experiments designed to explain observations and inspire theoreticians). This minisymposium presents an interdisciplinary spectrum of researchers working on three-dimensional water waves and focuses upon numerical simulations and experiments.

Experimental investigation and modeling of deep-water patterns of surface waves. **Diane Henderson** (Pennsylvania State University, USA) IC/MT3569/101

We present experiments in which we generate patterns of deep-water surface waves and investigate the geometric properties and the stability of these patterns. Craig & Nicholls (2002) found solutions to the fully nonlinear inviscid water wave equations whose periodic cell structure is rectangular. Iooss & Plotnikov (2006) found solutions for the same equations in different parameter regimes in which the periodic cell structure is hexagonal. We try to find these solutions in the experiments. We examine the stability of the patterns in the experiments and in asymptotic models, including the nonlinear Schrödinger (NLS) equation and a vector form of the NLS equation. In the inviscid models, the patterns are unstable to modulational perturbations. But we find that any amount of damping, of the right type, no matter how small, stabilizes this well-known instability both in the model equations and in the experiments. The NLS and VNLS equations, modified for damping, do a good job of predicting the evolution of the wave patterns with perturbations added. This work is joint with Harvey Segur, Joe Hammack, John Carter, Matt Patterson and others.

Computation of 3D interfacial waves and related flows. **Emilian Părău** (University of East Anglia, UK) IC/MT4066/101

Numerical computations of three-dimensional gravity and gravity–capillary interfacial waves are presented. Solutions of the fully nonlinear equations are calculated by boundary-integral equation methods. A configuration consisting of two superposed fluids bounded above by a free-surface is also considered. Further results are presented for time dependent free surface flows.

Numerical computations of 3D gravity-capillary waves. **Jean-Marc Vanden-Broeck** (University of East Anglia, UK) IC/MT1996/101

Three dimensional gravity capillary waves are considered. Accurate numerical computations are presented for the full Euler equations. The numerical methods are based on boundary integral equation techniques. Numerical evidence of three dimensional solitary waves is presented. The waves have decaying oscillations in the direction of propagation and monotonic decay in the direction perpendicular to the direction of propagation. Further results are presented for interfacial waves and time dependent free surface flows.

Numerical stability of a KdV equation with a negative forcing. **Sungim Whang** (National Institute for Mathematical Sciences, Republic of Korea), Jeongwhan Choi (Korea University, Republic of Korea) IC/MT2028/101

The waves at the free surface waves of a incompressible and invisid fluid in a two dimensional domains with horizontal rigid flat bottom with a small obstruction are considered. A time dependent KdV equation with a negative forcing is derived and studied both theoretically and numerically. The existence of a negative solitary-wave-like solution of the equation near the Froude number is proved and the numerical stability of the solution is also studied. The numerical stability of the positive both symmetric and unsymmetric solitary-wave-like solutions are also studied.

IC/MP64/103: Vortex dynamics.

Organiser: Hassan Aref (Danmarks Tekniske Universitet, Denmark)
Co-organiser: Paul Newton (University of Southern California, USA)

In 1858 Helmholtz published his seminal paper "Über Integrale der hydrodynamischen Gleichungen, welche den Wirbelbewegungen entsprechen", (J. reine u. angew. Math. **55**, 25–55), wherein he established his three laws of vortex motion in much the same way one finds them in any advanced textbook today. P. G. Tait later published an English translation, "On integrals of the hydrodynamical equations which express vortex motion", (*Phil. Mag.* **33**, (1867) pp.485–512). For the next century or so vortex dynamics matured as a subfield of fluid mechanics, always commanding at least a major chapter in treatises on the subject; e.g., Lamb's *Hydrodynamics* (1932) or Batchelor's *Introduction to Fluid Dynamics* (1967). In due course entire treatises were devoted to vortex motion; e.g., Poincaré's *Théorie des Tourbillons* (1893), Villat's *Lecons sur la Théorie des Tourbillons* (1930), Truesdell's *The Kinematics of Vorticity* (1954), and Saffman's *Vortex Dynamics* (1992). The range of applicability of Helmholtz's work grew to atmospheric and oceanographic flows, to all branches of engineering and applied science, aerodynamics in particular, and ultimately, to superfluids, including these days Bose–Einstein condensates. Today, one can scarcely imagine an investigation in fluid mechanics that does not invoke the role of vorticity or vortices in some way. Nevertheless, while vortices and vortex motion are ubiquitous, vortex dynamics retains a characteristic *flavor* deriving from its Lagrangian interpretation and from its frequently intuitive, *mechanistic* description of flow phenomena. At the same time vortex dynamics has consistently demanded rather sophisticated mathematical tools, in part because of the counterpoint between Lagrangian and Eulerian aspects that the field constantly demands. The minisymposium will bring leading experts in vortex dynamics to ICIAM and stimulate discussion across a broad range of mathematical fluid dynamics.

150 years of vortex dynamics. **Hassan Aref** (Danmarks Tekniske Universitet, Denmark) IC/MT1356/103

We are approaching the sesquicentennial of Helmholtz's seminal paper of 1858 in which the study of vortex motion was launched. In this lecture I will give a description of the laws of vortex motion. I will describe some of the models of vortices that have been studied and the wealth of phenomena that have been addressed using the theory of vortex motion. These include the totally erroneous notion of Kelvin that atoms are a kind of vortex motion in the ether, an idea that led to huge amounts of high quality work even though the application turned out to be misguided. Experiments by the American physicist Mayer on pattern formation by floating magnets were seized upon by Kelvin and his followers as illustrating the periodic table of the elements. Later, in 1911-12, T. von Kármán provided a remarkable application of the vortex dynamics of Helmholtz in his explanation of the structure and stability of bluff body wakes, an application that has stood the test of time. Some 35 years after that, through work by Onsager and Feynman, it was realized that superfluids could nucleate and sustain vortices that obeyed Helmholtz's dynamical equations. In 1979 the first experiments visualizing vortex arrays in rotating superfluid ^{4}He were reported. Understanding the geometry of the patterns formed by the vortices has been of ongoing interest. Recently, similar patterns have been observed in Bose-Einstein Condensates (BEC). Several highlights of the rich and sometimes bizarre history of vortex dynamics will be presented, with appropriate recognition of the topics to be presented by other authors in the minisymposium.

Self-similar collapse of the straight vortex-filament dodecapole. **Yoshi Kimura** (Nagoya University, Japan) IC/MT2711/103

The vortex dodecapole, the superposition of three equal-strength, orthogonal, vortex quadrupoles, was proposed by Rich Pelz and his co-workers as a candidate initial condition for a finite-time singularity in ideal hydrodynamics. In this paper, we examine the simplest model of the vortex dodecapole in which the vortex tubes are replaced with straight vortex filaments of infinitesimal thickness. It is demonstrated that this model permits a self-similar collaps solution which provides the time dependence of $\sqrt{t - t_c}$ where t_c, the collapse time, depends on the initial configulation. This time dependence agrees with the one observed in the direct numerical (pseudo spectral) simulations of the vortex dodecapole.

(This work is a part of collaboration with Rich Pelz who passed away suddenly in 2002.)

Point-vortex models of bluff body wakes. **Mark Stremler** (Virginia Tech, USA) IC/MT3080/103

When a two-dimensional bluff body wake is modeled as two oppositely-signed point vortices in a singly periodic strip, any choice of vortex positions gives a uniformly translating relative equilibrium. In the case of the staggered Kármán street, the wake translates along its length, and adjacent co-moving points (i.e., stagnation points in a frame moving with the vortices) are joined by streamlines. For small deviations from this ideal case, however, the wake translates obliquely, and the streamline structure becomes more intricate. Fluid entrained in the wake can be wrapped around many of the vortices before passing through to the other side. I will discuss the bifurcations that occur in the streamline topology of obliquely translating vortex streets and the influence of this structure on mixing in wakes.

The Kármán vortex street appears consistently in the wakes of rigid bluff bodies. If the body is instead free (or forced) to oscillate, the resulting wake structure can be much more exotic, with three or more vortices shed per period. I will present relative equilibrium configurations of singly periodic point vortex systems as models of these exotic wakes. When three vortices are shed per period, the possible configurations can be determined systematically. The focus here will be on those configurations that translate along the wake. The streamline topology in various exotic wake models will also be discussed.

Asymmetric equilibria via Brownian ratchets. **Paul Newton** (University of Southern California, USA) IC/MT1351/103

We formulate the problem of finding N-vortex equilibria in terms of the linear algebra problem $A\vec{\Gamma} = 0$, where A is an MxN configuration matrix whose entries are made up of inter-vortical distances, and $\vec{\Gamma} \in R^N$ is the vector of vortex strengths. In order for an equilibrium to exist, A must be rank-deficient, and the dimension of the nullspace corresponds to the number of free parameters available in choosing the vortex strengths. We randomly place N points in the plane, perform a singular value decomposition on A, and use the smallest singular value as a 'ratchet'. At each step, we allow the points to execute a random walk, and retain the new configuration only if the smallest singular value is reduced. This way, we can drive the configuration to an equilibrium (at least one singular value is zero) corresponding to an A matrix with any desired rank. The Frobenius norm allows us to measure the size of the equilibrium and distances between equilibria. We will also comment on uses of the pseudospectrum of A to understand the robustness of the configuration.

IC/MP234/103: **General solutions of fluid dynamics.**

Organiser: Victor Miroshnikov (College of Mount Saint Vincent, USA)

General solutions of fluid dynamics create a necessary mathematical framework for solving numerous boundary-value problems and bring understanding of general properties of fluid flows away from boundaries. The general solutions also build up a positive approach to the millennium problem on the existence of smooth solutions of the Navier–Stokes equations by constructing explicit solutions in the form of the Boussinesq–Rayleigh series, which provide a straightforward relation between formulations of unsteady problems in various dimensions. This minisymposium focuses on new developments in analytical, symbolic, and numeric algorithms for computing the general solutions of the Navier–Stokes, Stokes, and Oseen equations, considers applications of the general solutions for creeping flows, Poiseuille flows, and flows away from boundaries, and also addresses possible generalizations of the general solutions.

General solutions of the Navier–Stokes equations in various dimensions. **Victor Miroshnikov** (College of Mount Saint Vincent, USA) IC/MT2781/103

General solutions of the unsteady Navier-Stokes equations in one, two, and three dimensions are derived symbolically as the Boussinesq-Rayleigh series in a coordinate and continued numerically by parallel computing. The main results of this presentation are sorted in three groups. First, several exact theorems are proved for the Navier-Stokes equations and the Stokes equations since the differential and tensor recurrent relations may be written in the closed form. For instance, it is shown that flows away from boundaries may be decomposed into the following basic flows: the Couette flow, the Poiseuille flow, the Bernoulli flow and the Stokes flow. Second, symbolic existence theorems are obtained since computation, validation, and convergence of the free and forced general solutions of the Navier-Stokes equations is treated symbolically. Third, new numerical algorithms of evaluation, continuation, and visualization of multi-scale flow structures are developed. In three dimensions, the nested vortex pairs of the Poiseuille flow are visualized by stream surfaces and stream tubes formed by streamlines with constant integration times, which continue two-dimensional isocurves of the streamfunction. Comparison of mixing by the Poiseuille flow in one, two, and three dimensions is given through simulated animations, which display connections between flows in various dimensions.

General solutions of the Stokes equations and their applications. **Tirumalasetty Amaranath** (University of Hyderabad, India) IC/MT2617/103

The Stokes[1] equations have been one of the most extensively studied equations ever since Stokes discussed the resistance experienced by a slowly moving sphere. These equations have prompted mathematicians to develop a rich mathematical theory of slow, viscous flows which have benefited both scientists and engineers alike. There are numerous sphere theorems and solutions in literature which provide simple formulae for calculating physical quantities like drag and torque experienced by a sphere starting from Lamb's[2] solution till a recent solution of Stokes equations due to Palaniappan *et al.*[3]. We review the applications of the solution due to Palaniappan *et al.*[3], which we showed is a complete general solution, for the problem of an arbitrary Stokes flow past a sphere under different boundary conditions. The earliest formula for drag and torque acting on a sphere in an unbounded arbitrary Stokes flow was given by Faxen[4]. Such formulae have also been derived using the solution proposed in[3]. We also discuss another complete general solution of Stokes equations proposed by us, which is suitable for discussing the problem of an arbitrary Stokes flow involving plane boundaries. Payne and Pell[5] derived a formula for drag on an arbitrary body in an axisymmetric flow. An analogous result was obtained by Lawrence and Weinbaum[6] who calculated the force on an arbitrary axisymmetric body in an oscillatory motion. Although some methods have been derived earlier to develop exact solutions for axisymmetric bodies of different shapes, there seems to be no general method, albeit approximate, which gives the solution for the problem of non-axisymmetric Stokes flow for arbitrary shaped bodies, even for the simple case of an ellipsoid. A numerical method has been suggested by us to solve the problem of an arbitrary Stokes flow past a body of arbitrary shape.

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[6] Lawrence, C.J. and Weinbaum, S.; The force on an axisymmetric body in linearized time-dependent motion: a new memory term. J. Fluid Mech., Vol.171, 1986, pp.209–218.

General solutions of the Oseen equations. **B. Sri Padmavati** (University of Hyderabad, India) IC/MT2620/103

Flows at low Reynolds numbers are governed by the Stokes[1] equations. However these equations do not provide a satisfactory explanation of Stokes paradox; i.e., in explaining the validity of these equations at sufficiently large distances from the boundary. Oseen[2] modified Stokes equations by including a linearized convective term to them to explain it. These equations are known as Oseen equations. Lamb[3] proposed solutions of both Stokes and Oseen[2] equations. However Lamb's solution of Oseen equations which is commonly used is not adequate to represent all solutions of Oseen equations.

We shall discuss some results pertaining to divergence free vector fields which are relevant to Oseen equations and present a solution of Oseen equations. We also discuss some other previously known solutions of Oseen equations. We explain the merits of the new solution and highlight its advantages. We further show that it is a general solution, in the sense that, every other solution of Oseen equations can be represented in the form given by this new solution.

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Explicit description of isotropic tensor of high rank using polyadics for microhydrodynamics. **Teruo Kumagai** (Tokyo University of Science, Japan) IC/MT34/010

The purpose of this paper is to describe explicitly the isotropic tensor of high rank in three-dimensional space using the polyadic algebra for the recent continuum mechanics such as microhydrodynamics. The derivation of the Navier–Stokes equation for viscous flows needs an explicit description of a relation between strain and stress under the assumption of slight deformations and isotropic properties of the fluids. The strain–stress relation has already been derived using the isotropic ten-

sor of the rank up to 4. However there are left rooms to derive the isotropic tensor of the higher rank than 4. In this paper the isotropic tensor of the high rank is derived using the polyadic algebra. The polyadic, the direct product of unit vectors, denotes merely a combination of unit vectors, but is effective to represent the tensor for the transformation of coordinates. The isotropic property of fluids means the invariable property of the tensor for the rotation of the coordinates. The polyadic expression represents the tensor of rank n as the summation of combinations of unit vectors. For example n=0,1,2,3 and 4 means a scalar,a vector,a dyadic,a triadic and a tetradic respectively. The isotropic tensor of the high rank with even number is concluded to be described explicitly as the summation of combinations of the Kronecker delta, while the isotropic tensor of the high rank with odd number is concluded to be described as the summation of both of the Kronecker delta and the Edington epsilon. For example the isotropic tensor of rank 4 is described explicitly as the summation of three kinds of products of the Krönecker delta. This equation leads directly to the Navier–Stokes equation and the basic equtaion for microhydrodynamics.

IC/MP224/103: Mathematical analysis of the Euler equations and its applications.

Organiser: Hisashi Okamoto (Kyoto University, Japan)

The Euler equations are the governing equations of incompressible inviscid fluid motion. Mathematical results on the Euler equations are fewer than those of the Navier–Stokes equations. However, they are sources of many interesting phenomena such as vortex filaments, vortex sheets, and possible singularities. From a mathematical viewpoint these are far from well-understood, despite intensive numerical simulations. The present mini-symposium summarizes the current status of the mathematical study on the Euler equations and related equations.

On the Lagrangian dynamics for the 3D incompressible Euler equations. **Dongho Chae** (Sungkyunkwan University, Republic of Korea) IC/MT1504/103

In this talk we discuss the dynamical behaviors along the particle trajectories for some quantities of the 3D inviscid incompressible fluids. We construct ordinary differential equations satisfied by scalar quantities composed of spectrum of the deformation tensor, the hessian of the pressure and the direction field of the vorticity, and discuss the dichotomy between the finite time singularity and the long time behaviors of the various scalar quantities.

A personal survey on similarity solutions of Euler's equations. **Hisashi Okamoto** (Kyoto University, Japan) IC/MT2094/103

In this talk, I will survey some exact solutions of Euler's equations of inviscid incompressible fluid. They are obtained as solutions to some equations which are simpler than Euler equations. Those simplified equations include the Proudman-Johnson equation, equations for axisymmetric flows, and that for von Kármán's swirling flows. Since the velocity field of those solutions do not decay at infinity, their properties may not have a direct physical implication. But, if used locally in space region, they reveals interesting features and are helpful to understanding real flow phenomena. In this sense, reviewing a current status would not be uninteresting to application oriented scientist as well as mathematicians. I will begin with the issue of existence/non-existence of blow-up solutions, and then I will give some remarks concerning the role of the convection and stretching terms. It will be revealed that the convection terms prevent the solutions from blowing up. I then show some numerical experiments, from which conjectures are derived.

Blow-up and regularity problems of hypoviscous fluid equations. **Koji Ohkitani** (The University of Sheffield, UK) IC/MT2198/103

In this work, we treat generalised incompressible fluid equations with modified dissipativity. We consider specifically modifications of 1D Burgers and 3D Navier-Stokes equations, where the Newtonian viscosity is replaced with hypoviscous term $-\nu(-\triangle)^{\alpha}$, $(0 < \alpha < 1)$. The latter equations read with standard notations

$$\frac{\partial \boldsymbol{u}}{\partial t} + (\boldsymbol{u}\cdot\nabla)\boldsymbol{u} = -\nabla p - \nu_{\alpha}(-\triangle)^{\alpha}\boldsymbol{u},$$
$$\nabla\cdot\boldsymbol{u} = 0.$$

After reviewing some previous works on the subject, we will be particularly interested in the case $\alpha = 1/2$, which lies just between the Euler and Navier-Stokes equations.

In one space dimension, we will show that the Burgers equation with $\alpha = 1/2$ will generally lead to blow up in finite time. In three dimensions, we will consider under what conditions the solutions to hypoviscous equations remain smooth and decay in time.

Analytical behavior of an incompressible flow in a porous media. **Diego Cordoba** (Consejo Superior de Investigaciones Científicas, Spain) IC/MT2199/103

Here we study the analytical structure of a mass balance equation in a porous medium. Detailed mathematical criteria are developed as diagnostics for self-consistent numerical calculations indicating non-formation of singularities.

IC/MP4402/105: Recent advances in vortex dynamics: applications.

Organiser: Denis Blackmore (New Jersey Institute of Technology, USA)

See minisymposium IC/MP520/107on page 527.

Scalar transport and conditional averaging in an annular swirling jet. **Jochen Fröhlich** (Universität Karlsruhe, Germany), Manuel García-Villalba (Universität Karlsruhe, Germany), Wolfgang Rodi (Universität Karlsruhe, Germany) IC/MT4117/107

The paper presents large eddy simulations of co-annular swirling jets into an open domain at practical Reynolds number. In each of the jets a passive scalar is introduced and its transport is computed. If the exit of the pilot jet is retracted strong coherent flow structures are generated. Average and instantaneous fields are discussed. They are compared with corresponding experimental data and very good agreement is found. Probability density functions of the scalar concentration and turbulent fluxes are determined to assess the mixing efficiency of the flow. A conditional averaging technique is devised and applied to velocity and scalars. These data show the strong impact of the coherent structures on the mixing process.

Vortical flow in thermo-acoustic devices. **Katsuya Ishii** (Nagoya University, Japan), Masahiro Ishigaki (Nagoya University, Japan), Shizuko Adachi (RIKEN, Japan), Kazuto Kuzuu (Nagoya University, Japan), Masahiro Ishigaki (Nagoya University, Japan) IC/MT4128/107

The thermo-acoustic spontaneous oscillation phenomenon plays an important role in a thermo-acoustic engine. This oscillation occurs in a long tube with large thermal gradient. The phenomena in a 2D closed long tube are investigated by the numerical calculation of the compressible Navier-Stokes equations, in which the center part of the tube wall is cold(T=Tc) and the side parts of tube wall and both end walls are hot(T=Th). While any oscillations are not observed when the temperature ratio(Th/Tc) is smaller than 7, we observe a spontaneous oscillation when the temperature ratio(Th/Tc) is larger than 9.1. In this oscillation, the center of tube is an antinode of velocity and the ends of a tube are nodes. The wide boundary layer is observed and the time averaged values of pressure and temperature are constant in the hot part of tube. On the other hand, the boundary layer is narrow and the averaged values of pressure and temperature are different in the cross section. We also observe vortical flow and additional pressure flucutuation in the cold part of tube. We analyze the oscillation mechanism in detail and discuss the relationship of the oscillation phenomenon and vortex motion in the cold part of the tube.

Aircraft-wake vortices: prediction and mitigation. **Frank Holzäpfel** (DLR Oberpfaffenhofen, Germany), Thomas Gerz (DLR Oberpfaffenhofen, Germany) IC/MT4358/107

As an unavoidable consequence of lift, aircraft generate a pair of counter-rotating vortices, the so-called wake vortices. These vortices may exert a serious danger on following aircraft if the separation between leading and following aircraft is not sufficient. The incentive of today's wake vortex research still rests on the empirically motivated separation standards between consecutive aircraft introduced in the 1970s. These aircraft separations fix the capacity of congested airports in a rapidly growing aeronautical environment.

Two approaches are addressed that aim at increasing airport capacity without compromising safety. One approach is to directly impact wake vortex strength and stability by constructive measures at the aircraft wings. For example, suitable secondary wake vortex pairs are generated by differential flap settings that may trigger instrumental vortex instabilities. On the other hand, the dominant influence of meteorological parameters like turbulence, wind shear, and temperature stratification on wake vortex fate is utilized. The physical mechanisms that control the interaction of wake vortices with their environment in the meantime are largely understood. This knowledge constitutes the basis for predicting wake vortex behavior along the glide slope and dynamically adjusting vortex separations.

The current talk will present large eddy simulations that are employed within both approaches, the developped real-time wake vortex prediction model (P2P) and the Wake Vortex Prediction and Monitoring System (WSVBS) which has demonstrated its functionality at Frankfurt airport during winter 06/07.

Vortex-wake mitigation of an airfoil with winglets by active rudders. **Robert Schöll** (RWTH Aachen, Germany), Ralf Hörnschemeyer (RWTH Aachen, Germany), Sebastian Kauertz (Airbus Deutschland GmbH, Germany), Rolf Henke (RWTH Aachen, Germany) IC/MT4387/107

Wake vortices pose a hazard to airplanes and limit the capacity of airports. The wake vortex hazard has been a subject of research for over 30 years, yet the physical processes determining vortex decay are not fully understood. In the present investigation, experiments with a rectangular planform wing are conducted with the goal of influencing and mitigating the vortex wake by the generation of additional vortices. The experiments are carried out in a water towing tank, where two-component particle image velocimetry is used as the measurement method. This setup allows the measurement of the wake up to 40 wing spans downstream of the model.

The model is equipped with ailerons and winglet-integrated rudders, which can be set up to create a system of multiple trailing vortices. By setting appropriate deflection angles, an inherently unstable vortex system can be created, which breaks down considerably faster than the system produced by a clean wing configuration. Through stability analysis, frequencies can be identified at which short wave instabilites develop. The rudders integrated in the winglets are then oscillated at those frequencies with the aim of fostering short wave instabilities, leading to accelerated decay of the vortex system. After a modification of the model, it is possible to oscillate the ailerons as well.

Preliminary results show that the wake is influenced much more effectively when both ailerons and winglet rudder are oscillated, as compared to the case with rudder oscillation only.

IC/MP129/106: Mathematics and computations of complex flows.

Organiser: Traian Iliescu (Virginia Tech, USA)
Co-organiser: Anastasios Liakos (United States Naval Academy)

Complex flow phenomena occur in many areas of the sciences and engineering. In turn, they give rise to many interesting themes of fluid dynamics such as high Reynolds-number flow and large-eddy simulation for Newtonian fluids and high Weissenberg-number flow for viscoelastic fluids. Applications of these areas include, amongst many others, energy consumption optimization and global climate change estimation, polymer-processing operations (extrusion, injection molding), and sustained plasma confinement for controlled thermonuclear fusion and liquid-metal cooling of nuclear reactors respectively.

This minisymposium will focus on the modeling, analysis, and simulation of phenomena occurring in the flow of the aforementioned fluids and on underlying questions of numerical analysis and computational issues. Thus, it will be of interest to a broad audience of applied mathematicians, numerical analysts, and computational scientists.

Advances in MHD flow simulation. **Amnon Meir** (Auburn University, USA), Paul Schmidt (Auburn University, USA), Kang Jin (Auburn University, USA) IC/MT188/106

Magnetohydrodynamics (MHD) is the theory of the macroscopic interaction of electrically conducting fluids with a magnetic field. It is of importance in connection with many engineering problems such as plasma confinement, liquid-metal cooling of nuclear reactors, the CZ crystal growth process, and electromagnetic casting.

In the viscous incompressible case, MHD flow is governed by the Navier-Stokes equations and the pre-Maxwell equations giving rise to challenging problems of mathematical analysis and numerical approximation. We will discuss recent advances in MHD flow simulation.

Mathematical issues concerning the Boussinesq approximation for thermally coupled viscous flows. **Paul Schmidt** (Auburn University, USA), Jesus Ildefonso Diaz (Universidad Complutense de Madrid, Spain), Jean-Michel Rakotoson (Université de Poitiers, France) IC/MT289/106

The flow of a viscous, heat-conducting fluid under the force of gravity is governed by a system of balance equations for momentum, mass, and energy. In the so-called Boussinesq approximation, this system reduces to the Navier–Stokes equations for an incompressible fluid, coupled to a semilinear heat equation; the main coupling terms are buoyancy and viscous heating. Frequently, the latter is negligible, in which case the resulting initial-boundary value problems are well posed in the same sense as for the classical Navier–Stokes equations without thermal coupling. However, in situations where viscous heating cannot be neglected, well-posedness is an open question. We analyze the ensuing mathematical issues and present preliminary results for a simplified model.

Mathematical modelling and numerical simulations in blood rheology. **Adelia Sequeira** (Universidade Técnica de Lisboa, Portugal) IC/MT4360/106

Blood is a multi-component mixture with complex rheologic characteristics which interacts both mechanically and chemically with vessel walls, giving rise to complex fluid-structure interaction models whose mathematical analysis is still incomplete and which are difficult to simulate numerically in an efficient manner. Experimental investigations over many years show that blood flow exhibits non-Newtonian behaviour such as shear-thinning, viscoelasticity, thixotropy and yield stress and its rheology is influenced by numerous factors including plasma viscosity, rate of shear, hematocrit, level of erythrocytes aggregation and deformability. Hemodynamic analysis of blood flow in vascular beds and prosthetic devices requires the rheological behaviour of blood to be characterized through appropriate constitutive equations relating the stress to deformation and rate of deformation.

In this talk we present a short overview of some constitutive models that can mathematically characterize the rheology of blood and some numerical simulations to illustrate its phenomenological behaviour. Using a mesoscopic lattice Boltzmann flow solver for non-Newtonian shear thinning fluids, we present a recent three-dimensional numerical study of the dynamics of leukocytes rolling and recruitment by the endothelial wall, based on in vivo experimental measurements in Wistar rat venules. Preliminary numerical results obtained for a comprehensive model of blood coagulation and clot formation, that integrates physiologic, rheologic and biochemical factors will also be presented. The corresponding three-dimensional simulations were obtained for a shear-thinning blood model using a finite volume semi-discretization in space and a three-stage Runge-Kutta time integration method.

On finite-element variational multi-scale methods for incompressible turbulent flows. **Volker John** (Universität des Saarlandes, Germany), Adela Kindl (Universität des Saarlandes, Germany) IC/MT3486/106

Variational Multiscale (VMS) Methods are a new approach for the simulation of turbulent flows. Their key feature consists in the application of a turbulence model only to so–called resolved small scales which are defined by appropriate projections. This is in contrast to the classical Large Eddy Simulation (LES) where the turbulence model is applied to all resolved scales and the resolved scales are defined by spatial averaging.

The parameters of a VMS method are the turbulence model and the spaces for the large scales and the resolved small scales.

There are several ways for the realization of a VMS method in the context of finite element discretizations. The talk gives an overview on Finite Element VMS methods and numerical examples will be presented to compare the different approaches.

IC/MP129/106: Mathematics and computations of complex flows. #2

Organiser: Traian Iliescu (Virginia Tech, USA)
Co-organiser: Anastasios Liakos (United States Naval Academy)

(For abstract, see session #1 above.)

Finite-element method for viscoelastic fluid flows. **D Sandri** (Université Lyon 1, France) IC/MT2806/106

In this minisymposium we discuss the finite element (FE) method for the approximation of viscoelastic fluid flows. We consider the approximation of fluid flows obeying the Oldroyd model and particularly we study the purely viscoelastic case, the so-called Maxwell model, important in practice.
For the numerical approximation of the Maxwell model we study two kinds of methods : a method using a technique of splitting and usual FE methods based on finite element spaces satisfying inf-sup conditions relating tensor and velocity.

We also present numerical results for these methods and we discuss their stability.

Simulation of flow-induced microstructure development in liquid-crystal polymeric materials. **Christopher Cox** (Clemson University, USA) IC/MT3694/106

Liquid crystal polymers are found in commercial applications (e.g., Dupont Kevlar) and natural materials (e.g., spider silk). There is wide-spread interest in gaining deeper understanding of the flow properties of these fascinating and complex materials.
The goal of this effort is to simulate flows of liquid-crystalline polymer materials using tensor-order constitutive equations formulated by Rey and coworkers. Of particular interest is the development of textural effects and their influence on stress growth. The system of nonlinear partial differential equations governing the variation of (scalar, vector, and 2nd-order tensor) dependent variables will be described. Then the finite element formulation for this system will be discussed. Solutions under various flow conditions will be presented, beginning with simple test cases. Some comparisons to experimental results will also be provided.

This talk summarizes work conducted jointly by Professors Amod Ogale and Barr von Oehsen at Clemson University and Alejandro Rey at McGill University, Clemson University graduate students Edward Duffy and Santanu Kundu, and the speaker.

This work is supported primarily by the ERC program of the National Science Foundation under Award Number EEC-9731680.

Breaking complexity in fluid-structure interaction problems. **Georges-Henri Cottet** (Université Grenoble I, France) IC/MT3979/106

The main challenge in fluid-structure interaction problems comes form the necessity to combine models that are inherently different. A typical example is the dynamic of a living cell, which combines flow models inside the cell, elastic properties on the membrane and biochemical processes on the membrane and inside the cell.

From the numerical point of view, a common approach is to associate finite element-element type models for the fluid part with Lagrangian description of the elastic media. However these solutions are hard to implement, especially for 3D dynamics, and time-consuming. An alternative approach is to embed the whole system in a single Eulerian approach for which finite-difference algorithms are very cheap including for 3D complex behaviors. The fluid/structure interface is implicitly captured with a level-set method. Elastic properties are also formulated in terms of level-set functions. We will describe this approach and show some ongoing work in our group concerning applications in biomechanics, engineering and graphics animation.

Grid-filter models for large-eddy simulation. **Roland Bouffanais** (École Polytechnique Fédérale de Lausanne, Switzerland), Michel Deville (École Polytechnique Fédérale de Lausanne, Switzerland) IC/MT4014/106

A new interpretation of approximate deconvolution models (ADM) when used with implicit filtering as a way to approximate the projective grid filter is presented. Consequently, a new category of subgrid models, the grid filter models (GFM) is defined. ADM appear as a particular case of GFM since only approximate deconvolution is achieved. GFM can be either used with the standard filtered Navier–Stokes equations or with the formulation commonly used with ADM. The latter formulation requires an additional assumption leading to an incomplete modeling of the subgrid scales.

Based on GFM and ADM using these two different formulations of the filtered Navier–Stokes equations, several large-eddy simulations of the flow in a lid-driven cubical cavity have been carried out using the spectral element method. Numerical results for Reynolds number Re $= 12\ 000$ are presented and compared with direct numerical simulation (DNS) results found in the literature. In addition, An under-resolved DNS has also been carried-out to prove that the under-resolution is effective.

It is proved that the deconvoluted formulation, usually used with ADM, leads to an under-dissipative character of the subgrid model and explains the need of additional dissipative terms. Conversely, when using the standard filtered formulation, no additional term is needed which is of great relevance considering the confined nature of the flow and the high-order numerical method used. These results show an improvement over standard ADM-based subgrid models for large-eddy simulation.

Work done in collaboration with M.A. Habisreutinger.

IC/MP3638/106: Complex flows: mathematics and computations.

Organiser: Traian Iliescu (Virginia Tech, USA)
Co-organiser: Anastasios Liakos (United States Naval Academy)

Complex flow phenomena occur in many areas of the sciences and engineering. In turn, they give rise to many interesting themes of fluid dynamics such as high-Reynolds number flow and large eddy simulation for Newtonian fluids and high Weissenberg number flow for viscoelastic fluids. Applications of these areas include, amongst many others, energy consumption optimization and global climate change estimation, polymer-processing operations (extrusion, injection molding), and sustained plasma confinement for controlled thermonuclear fusion and liquid-metal cooling of nuclear reactors respectively.

viscoelastic fluids. Applications of these areas include, amongst many others, energy consumption optimization and global climate change estimation, polymer-processing operations (extrusion, injection molding), and sustained plasma confinement for controlled thermonuclear fusion and liquid-metal cooling of nuclear reactors respectively.

This minisymposium will focus on the modeling, analysis, and simulation of phenomena occurring in the flow of the aforementioned fluids and on underlying questions of numerical analysis and computational issues. Thus, it will be of interest to a broad audience of applied mathematicians, numerical analysts, and computational scientists.

Optimality and uncertainty in CFD: what is the best simulation ?. **Pierre Sagaut** (Université Pierre et Marie Curie-Paris 6, d'Alembe, France) IC/MT195/106

Numerical simulation of complex flows is at the very heart of many theoretical and industrial problems. Here, the notion of flow complexity is associated to its sensitivity/dependency with respect to large number of physical and numerical parameters. Typical physical parameters are the non-dimensional numbers such as the Reynolds number, geometrical parameters (e.g., a solid body shape), but also all parts of the physical model such as parameters that appear in turbulence models. Numerical parameters are the initial condition and the numerical errors, etc.

In almost all cases of real engineering relevance, many physical parameters are not precisely known, some of them being totally unknown. The validity of turbulence models is also not fully mastered in such configurations. In addition, the influence of the numerical errors on the solution, and their nonlinear couplings with the physical models is not fully understood.

Therefore, CFD for complex configurations is still an art, since its requires a lot of heuristics and *know how*. The present talk will present some results obtained by the author and many collaborators dealing with the quantification of flow sensitivity with respect to numerical and physical uncertainties, and the search for an *optimal* computational setup. A key tool for this is the parametrization of the space of the solution spanned by the physical model and the numerical method. The sensitivity of the solution is then defined as the local Jacobian of the solution in this space. The response surface approach is used for that purpose, based on both the Kriging and the Polynomial Chaos methods. It will be shown that, in some case, the *true* solution (as obtained from wind tunnel experiments or Direct Numerical Simulation) does not belong to the space of possible solutions. The use of a surface response approach makes it possible to define the *best* or *optimal* solution, once a measure of the error, defined as some kind of distance between the computed and the reference solutions, has been defined. It will be shown that (as can be expected), different definitions of the error yield different *best* solutions. An interesting observation is that the error is a non-convex function which exhibits several local minima in most cases, rendering the search for the *best* computational domain a difficult task. In some practical cases, such as the flow around a 2D wing, it will be shown that heuristic values of the parameters of the turbulence model and the artificial viscosities in the Jameson scheme are observed to correspond to a local minimum of the error.

Another interesting output of the surface response approach, which does not rely on any linearization approximation, is that

it allows for the description of the space of possible solutions of the computational model through statistical indicators, such as pdf and exact error bars.

This work was done in collaboration with: Dr. J.C. Jouhaud, Dr. D. Lucor, Dr. Y. Meyers, Dr. M. Montagnac.

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[3] D. Lucor, C. Enaux, H. Jourdren, P. Sagaut; Multi-Physics Stochastic Design Optimization: Application to Reacting Flows and Detonation. submitted.
[4] D. Lucor, J. Meyers, P. Sagaut; Sensitivity analysis of LES to subgrid-scale-model parametric uncertainty using Polynomial Chaos. submitted.

A two-level Smagorinsky model. **Traian Iliescu** (Virginia Tech, USA) IC/MT187/106

A two-level method for discretizing the Smagorinsky model for the numerical simulation of turbulent flows is proposed and analyzed. The two-level algorithm consists of solving a small nonlinear system of equations on the coarse mesh, and then using that solution to solve a larger linear system on the fine mesh. We demonstrate numerically that for an appropriate choice of grids, the two-level algorithm is significantly more efficient than the standard one-level algorithm.

Recent advances in the discretization of flows with shear-dependent viscosities. **Luigi Berselli** (Università di Pisa, Italy) IC/MT240/106

We consider non-newtonian flows with shear dependent viscosity, having in mind the classical Smagorinsky model but also more general flows capable of shear thinning/thickening. We prove some estimates for the space-time discretization showing optimal convergence for the time discrete problem.

IC/MP426/001: Fast solvers for saddle-point problems with applications in fluid dynamics.

Organiser: Guido Kanschat (Texas A&M University, USA)
Co-organiser: Maxim Olshanskii (Moscow State University, Russian Federation)

We review the state of the art of the development and analysis of efficient solution methods for saddle-point problems occurring in incompressible flow computations.

Several solution methods for Stokes and Navier–Stokes equations have been developed over the last decades. During the last years some convergence to block-preconditioning of the saddle-point problems could be observed. This type of preconditioners seems to offer the greatest flexibility with respect to the actual flow model (low/high Reynolds number, stationary/instationary, non-/Newtonian) and has been studied in a considerable amount of publications. The speakers of this minisymposium have been involved in these developments and in the application of this approach to various discretizations of flow problems. We will discuss the state achieved in analysis and application of these methods as well as future trends.

Symmetric indefinite preconditioners for saddle-point problems with applications to PDE-constrained optimization problems. **Walter Zulehner** (Universität Linz, Austria), Joachim Schöberl (RWTH Aachen, Germany) IC/MT2275/106

We consider large scale sparse linear systems in saddle-point form. A natural property of such indefinite 2-by-2 block systems is the positivity of the (1,1) block on the kernel of the (2,1) block. Many solution methods, however, require that the positivity of the (1,1) block is satisfied everywhere. To enforce the positivity everywhere, an augmented Lagrangian approach is usually chosen. However, the adjustment of the involved parameters is a critical issue. We will present a different approach that is not based on such an explicit augmentation technique. For the considered class of symmetric and indefinite preconditioners, assumptions are presented that lead to symmetric and positive definite problems with respect to a particular scalar product. Therefore, conjugate gradient acceleration can be used.

An important class of applications are optimal control problems. It is typical for such problems that the cost functional contains an extra regularization parameter. For control problems with elliptic state equations and distributed control a special indefinite preconditioner for the discretized problem is constructed which leads to convergence rates of the preconditioned conjugate gradient method that are not only independent of the mesh size but also independent of the regularization parameter. Numerical experiments are presented for illustrating the theoretical results.

Performance of saddle-point preconditioners in two practical settings. **Howard Elman** (University of Maryland, USA) IC/MT5023/106

Discretization of the incompressible Navier–Stokes equations and solution of the nonlinear algebraic equations by Newton or Picard iteration requires the solution of systems of equations with saddle point structure. We give an overview of preconditioning methods for these problems, and we demonstrate the effectiveness of the methods in several practical settings. In particular, we have integrated them into a general purpose finite element package, MPSalsa, developed at Sandia National Laboratories, and we show that they are very efficient for solving models of enclosed flow and flows over obstacles in two and three dimensions. We demonstrate the effective implementation of the ideas in a large-scale parallel setting, using multigrid for component problems. Moreover, we show improvements in performance (with speedups of factors of five to ten for large problems) achieved in comparison to more traditional methods used for incompressible flow, including the SIMPLE algorithm and domain decomposition strategies. Finally, we show that these methods can be used effectively to solve incompressible flow problems that arise in a model used to construct microfluidics devices for measuring the properties of mixing fluids.

Fast solvers for viscoelastic flows. **Daniel Loghin** (University of Birmingham, UK) IC/MT2768/106

Numerical simulations of viscoelastic flow problems require the solution of large, typically sparse, systems of equations which inherit the (highly) nonlinear coupling of the original PDE model. Recent approaches, such as the elastic viscous split stress (EVSS) methods, while allowing more flexibility and the treatment of complex rheological models come at the cost of increased problem size. At the same time, there is an evident lack of efficient solution techniques. In this work we introduce and analyze a class of implicit iterative solvers based on a Schur complement approach. The technique is based on identifying a suitable decoupling of the original system of PDE through an approximation to a Schur complement operator. We illustrate our approach on discretizations of EVSS formulations of Oldroyd-type fluid models.

Augmented Lagrangian approach for saddle-point problems with indefinite $(1,1)$-block. **Maxim Olshanskii** (Moscow State University, Russian Federation) IC/MT545/106

We discuss block preconditioners for a system of linear algebraic equations of saddle-point type having indefinite and not necessarily symmetric (1,1) block. The approach is based on considering an augmented system and a special multilevel method as an inner solver for a preconditioned Krylov subspace method. To explain convergence properties of the method we first prove bounds on the eigenvalues of the augmented (1,1) block. Next we consider the application of the method to solve a problem arising in the linear instability analysis for the Navier-Stokes equations. Several new results are proved for the Schur complement of the linearized Navier-Stokes equations. This provides further insight into the convergence properties of the approach.

IC/MP426/001: **Fast solvers for saddle-point problems with applications in fluid dynamics.** #2

Organiser: Guido Kanschat (Texas A&M University, USA)
Co-organiser: Maxim Olshanskii (Moscow State University, Russian Federation)

(For abstract, see session #1 above.)

Saddle-point preconditioners for higher-order discontinuous Galerkin discretizations of flow problems. **Guido Kanschat** (Texas A&M University, USA) IC/MT460/106

Non-symmetric H-matrix preconditioners for the Navier–Stokes equations. **Sabine Le Borne** (Tennessee Technological University, USA) IC/MT1039/106

The ability to solve large, sparse saddle point systems arising from the Navier–Stokes equations is critical to the success of numerical fluid flow simulations. Linear systems are typically solved by iterative methods, and their convergence can be accelerated by use of suitable preconditioners. A variety of preconditioning methods for saddle point problems has been significantly extended within the last decade. Several of these preconditioners are formulated in a general framework and require the solution of subproblems which, if solved exactly, imply the solution of dense linear systems of equations. A prominent example for such a subproblem is the solution of a Schur complement problem.

Hierarchical ($\mathcal{H}$-)matrices provide a powerful technique to compute and store approximations to dense matrices in a data-sparse format. In this talk, we will illustrate how to exploit $\mathcal{H}$-matrix techniques in the construction of efficient preconditioners for saddle point problems. We will conclude with numerical results for a variety of resulting preconditioners.

Preconditioning and convergence in the right norm. **Andy Wathen** (University of Oxford, UK) IC/MT1407/106

The Minimum Residual methods MINRES (for symmetric matrices) and GMRES (for non-symmetric matrices) are widely used for solving the large dimensional linear(ized) systems which derive from approximation of saddle-point (and other) problems. Almost universally preconditioning is used in an attempt to get convergence in a feasible computing time. One affect of the preconditioner with these methods however is to change the norm in which the residual is minimised.

In this talk we will show that appropriate block diagonal preconditioning for the Stokes problem not only guarentees mesh-independent convergence (as proved well over a decade ago in joint work with David Silvester) but also gives convergence in the natural norm for the problem ie. in the 'right' norm!

This is joint work with Howard Elman and David Silvester

Variations on pressure convection–diffusion preconditioners for saddle-point problems. **Raymond Tuminaro** (Sandia National Laboratories, USA) IC/MT1580/106

Pressure convection-diffusion (PCD) preconditioners introduced by Kay, Loghin, and Wathen have been successfully applied to several benchmark flow problems. This talk considers three algorithm variations. The first centers on the development of a new set of boundary conditions for the Poisson and convection-diffusion operators that must be defined for the preconditioner on the pressure space. The new boundary conditions are motivated by Fourier analysis of model flow problems. The second PCD variant is based on a block factorization that resembles the SIMPLE algorithm. The key advantage is that both approximate L and U factors can be employed cheaply within the preconditioner (as opposed to the standard method that uses only the U factor). The third variant considers the reuse of Krylov information between inner preconditioning solves.

Numerical results are given illustrating the benefits to the new variants on a variety of problems.

IC/MP692/106: **The Lagrangian-averaged Navier–Stokes alpha (LANS-α) turbulence model: theory, simulation, and comparison with related models.**

Organiser: Mark Petersen (Los Alamos National Laboratory, USA)

The LANS-α model is a sub-grid scale turbulence model that uses Lagrangian averaged velocity fields to address the turbulence closure. It modifies the nonlinearity of the Navier–Stokes equation, rather than the dissipation, resulting in a turbulence model without enhanced viscosity. LANS-α is a member of a hierarchy of equations developed using asymptotic methods on the Lagrangian in Hamilton's principle. These equations have desirable characteristics, such as conservation of energy and potential vorticity in the absence of dissipation, and Kelvin's circulation theorem.

The LANS-alpha model was introduced in Chen *et al.* (1998), and has since been tested in a variety of numerical simulations. In high Reynolds-number pipe flow, simulations matched observations of mean velocity over several orders of magnitude and showed that the LANS-α model could accurately describe turbulence over a wide range of scales. In forced isotropic turbulence in a three-dimensional periodic domain, the energy spectrum $E(k)$ was proportional to $k^{-5/3}$, as expected (Chen *et al.*, 1998). The LANS-α model was more accurate than a dynamic large-eddy simulation when measured against a reference solution from a high-resolution direct numerical simulation (Geurts and Holm, 2002). A quasi-geostrophic model, developed by Holm and Nadiga (2003), showed that the LANS-α can capture the qualitatively correct time-mean circulation

in the double-gyre problem at a resolution four to eight times courser than a traditional QG model. The LANS-α model was found to affect the baroclinic instability in a two-layer quasi-geostrophic model; it lowers the critical wavenumber, reduces the bandwidth of the instability, and preserves the value of forcing at the onset (Holm and Wingate, 2005).

The LANS-α model is now being tested in primitive equation ocean–climate models, where the gains in the resolution of small-scale processes must be weighed against the computational cost of the turbulence model.

A study of the Navier–Stokes-α model for 2D turbulence. **Evelyn Lunasin** (UC Irvine, USA), Susan Kurien (Los Alamos National Laboratory, USA), Mark Taylor (Sandia National Laboratories, USA), Edriss Titi (Weizmann Institute and University of California, Israel) IC/MT804/106

The Navier–Stokes-α sub-grid scale model of turbulence is a mollification of the Navier–Stokes equations in which the vorticity is advected and stretched by a smoothed velocity field. The smoothing is made by filtering the velocity field over spatial scales of size smaller than α. The statistical properties of the smoothed velocity field are expected to match those of Navier-Stokes turbulence for scales larger than α, thus providing a more computable model for those scales. For wavenumbers k such that $k\alpha > 1$, corresponding to scales smaller than α, there are three possible scalings of the energy spectrum, arising from three dynamical timescales in the model equations: one from the smoothed field, the second from the rough field and the third from a combination of the two. Using two-dimensional turbulence as the test case, we measure the scaling of the spectra from high-resolution simulations of the Navier-Stokes α-model, keeping all parameters other than α fixed. We show that the energy spectrum of the smoothed velocity field scales as k^{-7} in the enstrophy cascade regime, consistent with dynamics dominated by the timescale of the *rough* velocity field. This result implies that the rough velocity field plays a crucial role in the development of the smoothed field even though the latter is the purported model for the Navier–Stokes turbulence. This effect must be taken into account when performing accurate simulations of the α-model.

A new energy-conserving Lagrangian method for the rotating shallow water equations, derived using Voronoi diagrams in Hamilton's action principle. **Matthew Dixon** (Imperial College London, UK) IC/MT920/106

Geometric numerical methods seek to transfer powerful concepts in geometric mechanics to computational fluid dynamics. It is well known that the continuum LANS-α model is derived from Hamilton's action principle and the resulting flow has variational structure. A suitable class of numerical methods for the LANS-α model should also be derived from a discrete Hamilton's principle so that the discrete flow field too has variational structure.

In this talk, I shall present my research on the design of a new Lagrangian method for rotating shallow water with bottom topography which is derived from a semi-discrete Hamilton's action principle. The novel part is the use of a Voronoi diagram to represent the density field. This is dynamically reconstructed at each time step and therefore avoids mesh tangling problems encountered by many Lagrangian methods. This property together with the versatility of the Voronoi diagram makes this method attractive for the long-time simulations on the sphere required for modelling of the earth's climate. The action principle prescribes the form of the discrete gradient and divergence operators required for the semi-discrete shallow water equations to conserve energy. By choosing the form of the discrete curl operator, the semi-discrete divergence and potential vorticity equations are also derived. Potential vorticity is only conserved when the divergence of the discrete curl operator is zero, however. Numerical results of long-time shallow water simulations on an f-plane confirm that this method conserves mass (locally) and energy, and remains stable at larger time steps. We close this talk with a discussion of how this approach can be extended to the LANS-α model by considering the shallow water-α model.

Fluid and numerical stability in the LANS-α model. **Beth Wingate** (Los Alamos National Laboratory, USA) IC/MT4554/106

We present two stability results for the LANS-α model. The first result shows that the LANS-α model's regularization moves the baroclinic instability to lower wave numbers while preserving all the classical baroclinic instability theorems. The second result shows that the LANS-α model, for the fastest waves in climate models, can take a larger maximum allowable time step.

The LANS-α turbulence model in primitive-equation ocean modeling. **Mark Petersen** (Los Alamos National Laboratory, USA), Matthew Hecht (Los Alamos National Laboratory, USA), Darryl Holm (Imperial College London, UK), Beth Wingate (Los Alamos National Laboratory, USA) IC/MT4560/106

POP, the Parallel Ocean Program developed and maintained by Los Alamos National Laboratory, is widely used by the ocean and climate modeling community. Like all numerical models, computational time limits the spatial resolution at which POP can operate; standard climate simulations use grids of 0.5 to 1 degree in latitude and longitude. This resolution does not capture the motion of eddies at the Rossby radius of deformation, and thus lacks the correct energy cascade and heat transport at these scales. The Lagrangian-Averaged Navier–Stokes-α (LANS-α) model, developed by Darryl Holm and colleagues at Los Alamos, improves statistics such kinetic energy, eddy kinetic energy, and temperature profiles with a smoothed advecting velocity and an additional nonlinear term. I will discuss the implementation LANS-α in POP, and present results from a channel-domain experiment that is an idealization of the Antarctic circumpolar current.

IC/MP692/106: The Lagrangian-averaged Navier–Stokes alpha (LANS-α) turbulence model: theory, simulation, and comparison with related models. #2

Organiser: Mark Petersen (Los Alamos National Laboratory, USA)

(For abstract, see session #1 above.)

Regularization modeling of mixing in stratified turbulence. **Bernard Geurts** (Universiteit Twente, The Netherlands) IC/MT4724/106

The effects of stable and unstable stratification on the turbulent transport in a shear layer are quantified by monitoring global geometric properties of constant density surfaces, such as their area and wrinkling. The flow is simulated using direct and large-eddy simulation, in which regularization modeling for the subgrid scales in the momentum and the scalar equations is adopted and compared to dynamic subgrid modeling. The effects of high Schmidt number in the context of large-eddy simulation is investigated.

On the inertial subrange of symmetry-preserving regularization models for turbulent flow. **Roel Verstappen** (Rijksuniversiteit Gronigen, The Netherlands) IC/MT4727/106

Most turbulent flows cannot be computed directly from the (incompressible) Navier–Stokes equations because they possess too many scales of motion. In the quest for a dynamically less complex mathematical formulation, we consider symmetry-preserving regularizations of the convective nonlinearity. The regularized system should be more amenable to approximate numerically, while its solution has to approximate the low wave-numbers of the Navier–Stokes solution; *i.e.*, at least the first part of inertial subrange is to be approximated properly.

In this talk, we prove, using the arguments of Foias *et al.* (*CRAS I*, 333(5):499–504, 2001), that for any skew-symmetric regularization the energy flux through a wavenumber κ is nearly constant and, hence, independent of the viscosity and κ, throughout a certain range of wavenumber $\kappa_f \leq \kappa \leq \kappa_e$, where κ_f denotes the highest wavenumber of the forcing and κ_e can be estimated in terms of the solution of the regularized system. This rigorous result shows that for $\kappa_f \leq \kappa \leq \kappa_e$ the conditions prevailing in the inertial range for the energy cascade are strictly satisfied for any skew-symmetric regularization of the Navier–Stokes equations. A simple dimensional analysis gives then Kolmogorov's $-5/3$ spectrum.

Lagrangian coherent structures in atmospheric and ocean flows. **Jerrold Marsden** (California Institute of Technology, USA) IC/MT4801/106

We will report on progress towards understanding transport and entrainment processes in ocean and atmospheric flows. Special emphasis will be given to Hurricane dynamics. The computational methodology is based on Lagrangian Coherent Structures, a generalization of invariant manifolds to the time dependent context using George Haller's idea of locating ridges in the finite time Liapunov exponent field. In particular, Typhoon Nabi and Hurricane Katrina will be analyzed and Poincaré-Smale lobe dynamics will be shown to be a dominant transport mechanism.

Mathematical study of certain analytical sub-grid scale of turbulence. **Edriss Titi** (Weizmann Institute and University of California, Israel) IC/MT4806/106

In this talk I will discuss the subtleties and challenges in the mathematical study of the Navier-Stokes and Euler equations. Moreover, I will discuss recent developments in the mathematical study of certain analytical sub-grid scale models of turbulence.

IC/MP520/107: Recent advances in vortex dynamics: theory and computation.

Organiser: Denis Blackmore (New Jersey Institute of Technology, USA)
Co-organiser: Patrick Bontoux (Université Paul Cézanne Marseille, France)
Co-organiser: Chjan Lim (Rensselaer Polytechnic Institute, USA)

The last thirty years have witnessed an explosion of research innovations in vortex dominated flows ranging from Hamiltonian, nonlinear dynamics and classical differential equations analysis of vortex structures to state-of-the-art computational and experimental studies of vortex phenomena. These advances have had a profound effect on applications of fluid mechanics in science, engineering and industrial research, which have led to innovations in aircraft, ship and engine design, and have dramatically enhanced our understanding of ocean dynamics and meteorology, to name just a few areas.

An outstanding slate of distinguished researchers will describe an interesting variety of novel methods and approaches in vortex dynamics, and will discuss applications of their results to problems in science and engineering. The advances presented will embrace the analytical, computational, and experimental aspects of vortical flow research. This minisymposium is a continuation of a very successful series of minisymposia staged by the organizers and their colleagues at major conferences throughout the world over the last several years, the last of which was an embedded session at the GAMM Annual Meeting in Berlin in 2006.

Vortex phenomena in film-cooling flows. **Wolfgang Schroeder** (RWTH Aachen, Germany) IC/MT3745/107

The jet-in-a-crossflow problem is investigated using large-eddy simulations; i.e., the Navier–Stokes equations plus a set of transport equations for several species to simulate a non-reacting gas mixture are solved. Various density and velocity ratios of the outer flow and the injected jet are analyzed and the numerical results are compared with particle-image velocimetry measurements. Conclusions concerning the impact on the cooling efficiency are drawn.

Stability and transitions in fluid dynamics and geophysical fluid dynamics. **Shouhong Wang** (Indiana University, USA) IC/MT4108/107

I shall address in this talk the structure, its formation, its robustness/stability and transitions of fluid flows and geophysical fluid flows, focusing on the connections between the structure in the physical spaces and the dynamics of the flows. This is an important and challenge problem. I shall present some recent progresses, based on two recently developed theories: a geometric theory for incompressible flows and a dynamic bifurcation theory for nonlinear evolution equations. I shall present these theories together with examples on boundary layer separation and on dynamic bifurcation in fluid dynamics and geophysical fluid dynamics to demonstrate the main issues and ideas involved. In particular, I shall present how the Taylor vortices are formed in the Taylor-Couette-Poiseuille flow. This is joint work with Tian Ma.

Motion of integrable four-vortex points on sphere. **Takashi Sakajo** (Hokkaido University, Japan) IC/MT3447/107

We consider the motion of the four vortex points on a sphere when the moment of vorticity vector is zero, which is an integrable dynamical system. With the reduction method that is successfully developed by Aref and Stremler in the integrable planar 4-vortex problem, we give a complete description of the integrable system. We also investigte whether the fully or partial self-similar collapse of the four vortex points is possible or not.

The spherical integrable four-vortex problem is of significance more than just an unsolved problem. In general, a periodic orbit of the N vortex points defines a two-dimensional homeomorphism on the sphere with N fixed points, which is called the N-braids. According to Thurston-Nielsen theory, the N-braids is topologically classified into three types: periodic, pseudo-Anosov(pA) and reducible. The pA map induces a complex behavior, known as the topological chaos. Since it is mathematically proved that the 3-braid on sphere is always periodic, we need to consider the more than three vortex points

in order to obtain the pA N-braids. On the other hand, while it is generally difficult to find a periodic orbit, the integrable four-vortex problem provides us with infinitely many periodic orbits, which helps us find the pA braids. In the present talk, we examine the topological structure of the periodic orbits and observe the chaotic particle mixing due to the pA 4-braids.

Invariant tori in perturbed three-vortex motion. **Denis Blackmore** (New Jersey Institute of Technology, USA), Lu Ting (Courant Institute, NYU, USA), Omar Knio (Johns Hopkins University, USA) IC/MT4357/107

The motion of three-point vortices in an ideal fluid in a plane comprises a Hamiltonian dynamical system that is completely integrable, so it exhibits numerous periodic cycles and quasi-periodic orbits on invariant tori. Certain perturbations of three-vortex dynamics in a plane, such as three-vortex motion in a half-plane, are also Hamiltonian, but not completely integrable. Yet these perturbed systems may still have periodic trajectories and invariant tori close to those for the unperturbed dynamics. Extending recent work by the authors (to appear in J. Math. Phys.), invariant tori approximating those for the unperturbed system are located and analyzed using a combination of classical analysis, asymptotics, and KAM theoretical methods. The results and approximation methods used are then illustrated via simulations for several perturbations of three vortex dynamics such as three vortices in a half-plane, the restricted four vortex problem in the plane, and three coaxial vortex rings.

IC/MP520/107: Recent advances in vortex dynamics: theory and computation. #2

Organiser: Denis Blackmore (New Jersey Institute of Technology, USA)
Co-organiser: Patrick Bontoux (Université Paul Cézanne Marseille, France)
Co-organiser: Chjan Lim (Rensselaer Polytechnic Institute, USA)

(For abstract, see session #1 above.)

Dynamics of planar vortex clusters with binaries. **Lu Ting** (Courant Institute, NYU, USA), Omar Knio (Johns Hopkins University, USA), Denis Blackmore (New Jersey Institute of Technology, USA) IC/MT3520/107

We study planar motion of N point vortices with two close together relative to their distance from the others, and call such a pair of vortices a *binary*. It is shown that the leading order representation of the dynamics can be viewed as being comprised of $(N-1)$ vortices, with the binary treated as a single vortex located at its center of vorticity. In particular, the effects of the fast rotaion of the binary appear as higher order corrections. This leads to a two-time and two-length (multiple) scale perturbation problem. We begin by applying this multipe scale scheme to the analysis of a system in the case $N = 3$ with a binary to describe various aspects of the motion. The analysis is then extended to the study of N vortex problems (viewed as perturbations of three vortex dynamics) for systems containing one or more binaries. In addition, the analytical methods developed are used to interpret dynamical features observed in several numerical examples involving three or more vortices with clusters that include binaries.

Decomposing the platonic-solid vortex equilibria on the sphere. **Paul Newton** (University of Southern California, USA) IC/MT3502/107

We will describe a new method of finding and classifying N-vortex relative equilibrium configurations on the sphere. The problem is formulated as one in linear algebra, $A\vec{\Gamma} = 0$, which is obtained by requiring that all intervortical distances remain fixed. One must find a basis set for the nullspace of a non-normal ($A^TA \neq AA^T$) configuration matrix A. The vector $\vec{\Gamma} \in R^N$ is the vector of vortex strengths. The method is described for the 5 Platonic solid configurations on the sphere, where a point vortex is placed at each vertex. The full set of vortex strengths which make these configurations equilibria is surprisingly rich, as obtained by using the singular value decompostion of the configuration matrix A. The talk is based on M. I. Jamaloodeen, P.K. Newton, 'The N-vortex problem on a rotating sphere. II. Heterogeneous Platonic solid equilibria', Proc. Roy. Soc. A, 462, (2006), 3277-3299.

Statistical equilibrium predictions for quasi-2D flows with complex boundaries. **Chjan Lim** (Rensselaer Polytechnic Institute, USA) IC/MT3587/107

Equilibrium statistical mechanics have been applied to macroscopic flows using formulations - canonical or microcanonical in the kinetic energy of the flow - based on either a vortex gas, lattice or spectral representation of vorticity, predominantly in simple domains with either no boundaries or periodic boundary conditions. Most experiments however are performed in no-slip boxes. Furthermore, many interesting phenomena in geophysical flows are found in the category of coupled fluid - container systems such as the those concerning the super-rotation of a barotropic fluid coupled through a torque mechanism to a massive rotating sphere. We give a statistical equilibrium theory - wherein the kinetic energy is not a Hamiltonian and the angular momentum of the fluid can vary - for this class of coupled flows with complex boundaries and show how to obtain predictions of phase transitions under these non-standard conditions. Only the smallest possible set of constraints are retained in our new formulation - energy, total circulation, enstrophy - because complex boundary conditions implies that higher vorticity moments and angular momentum are not conserved even in the absence of viscosity.

Scaling of space-time modes with Reynolds number in two-dimensional turbulence. **Nicholas Kevlahan** (McMaster University, Canada) IC/MT4242/107

It has been estimated that the number of spatial modes (or nodal values) required to uniquely determine a two-dimensional turbulent flow at a specific time is finite, and is bounded by $Re^{4/3}$ for forced turbulence and Re for decaying turbulence. The usual computational estimate of the number of space-time modes required to calculated decaying two-dimensional turbulence is $\mathcal{N} \sim Re^{3/2}$. These bounds neglect intermittency, and it is not known how sharp they are. In this paper we use an adaptive multi-scale wavelet collocation method to estimate for the first time the number of space-time computational modes $\mathcal{N}$ necessary to represent two-dimensional decaying turbulence as a function of Reynolds number. We find that $\mathcal{N} \sim Re^{0.9}$ for $1\,260 \leq Re \leq 40\,400$ over many eddy turn-over times, and that temporal intermittency is stronger than spatial intermittency. The spatial modes alone scale like $Re^{0.7}$. The β-model then implies that the spatial fractal dimension of the active regions is 1.2, and the temporal fractal dimension is 0.3. These results suggest that the usual estimates are not sharp for adaptive numerical simulations. The relatively high compression confirms the importance of intermittency and encourages the search for reduced mathematical models of two-dimensional turbulence (e.g. in terms of coherent vortices).

IC/MP280/107: Particle transport by the atmosphere.

Organiser: Robert McKibbin (Massey University, New Zealand)
Co-organiser: Shigeo Kimura (Kanazawa University, Japan)

Talks and discussion will take place on windborne particle transport, dispersion, trapping and deposition (volcanic ash, pollen, pollution, yellow sand, spray droplets, snow, etc.). Often, these application areas are discussed at specialist conferences on, for example, volcanology, or environment, or horticulture, etc. This minisymposium will bring these researchers together to discuss methods, techniques and share good practice in solving these complex geophysical problems.

Topics and applications include particle transport/dispersion/trapping; dispersion in forest canopies; models of tephra dispersal/volcanic ashfall; yellow sand; numerical simulation of pollutant transport in the atmosphere; droplet motion and sprays; particle tracking models; wildfires; snow dispersion.

Sedimentation of volcanic particles. **Costanza Bonadonna** (Université de Genève, Switzerland), Jeremy Phillips (University of Bristol, UK) IC/MT3056/107

Particle fallout is one of the main products of explosive volcanic eruptions and occurs after material has been explosively ejected from a vent producing an eruption column, which is a buoyant plume of particles (tephra) and gas rising typically to stratospheric levels. Tephra can be transported in the atmosphere for significant distances, leading to dispersal over thousands of square kilometers around the volcano, and is a significant hazard causing respiratory problems to human and animals, serious damage to buildings and affecting economic sectors such as agriculture and tourism for many years after an eruption. The study of tephra dispersal represents an important aspect of hazard mitigation but it also provides important insights into eruptive-column dynamics. As a result, the study of tephra sedimentation has followed two main directions: (i) the detailed investigation of the dynamics of tephra fallout and (ii) the mitigation of tephra hazards. The first approach tries to capture the complex processes of particle transport in volcanic plumes and in the atmosphere, using a mixture of deterministic and probabilistic methods, whereas the second approach focuses on reliable mapping of tephra dispersal using predominantly probabilistic methods. In this talk we review the formulation of existing models of tephra dispersal, and discuss recent advances in computation methods that have allowed development of more sophisticated formulations. In particular, we identify important processes such as particle aggregation and the effects of particle shape on settling velocity that are currently poorly understood, and identify key areas of future development, including integration with remote sensing methods to improve model validation.

High-resolution numerical simulations of buoyant plumes from intense heat sources and implications for particle transport. **Philip Cunningham** (Florida State Universty, USA) IC/MT2616/107

Buoyant plumes arise routinely in a wide variety of geophysical contexts, examples of which include plumes from wildfires and volcanoes; many such plumes are important for the transport of particles in the atmosphere. Much information about the macroscale aspects of buoyant plumes can be obtained by application of the so-called entrainment hypothesis, which assumes that the flow is self-similar well above the source and that the mean inflow across the edges of the plume is proportional to the mean vertical velocity along the plume centerline. Although this approach has largely been successful in describing plume behavior over a wide range of scales, experimental estimates of the entrainment rate in buoyant plumes have varied widely, apparently due to the role of the coherent vortices that are generated in the near-source region and that impact entrainment in the far field. Moreover, for plumes from intense heat sources in the presence of nonuniform ambient flows, the assumption of similarity may break down and numerical solution of the governing equations is required. Well-resolved numerical simulations of thermal plumes are still somewhat rare, however, and a detailed understanding of the turbulent dynamics of buoyant plumes remains elusive.

In this talk, the structure and dynamics of buoyant plumes arising from isolated heat sources both in calm conditions and in the presence of an ambient cross flow are examined using a large-eddy simulation (LES) model. The basic structure and behavior of the simulated plumes will be presented, along with the dependence of this structure and behavior on parameters such as the speed of the ambient cross flow and the intensity of the heat source (i.e., the buoyancy forcing). Results from the LES model illustrate the role and significance of coherent vortices in plume dynamics. Indeed, in the presence of an ambient flow, the interaction between the vorticity in the cross flow boundary layer and the buoyancy generated vorticity in the plume results in the generation of several types of coherent vortical structures that dominate the structure and behavior of the plume. Finally, the dynamics of buoyant plumes in the presence of more complex environmental flows will be considered, such as the case of buoyant plumes interacting with density currents. The implications of the results for particle transport in the atmosphere will be addressed.

Organized flow structure and turbulent diffusion in a forest canopy. **Shigeo Kimura** (Kanazawa University, Japan) IC/MT1222/107

The wind velocities and turbulent properties in a plantation of *Quercus variabilis* Blume and *Quercus serrata* Murray belonging to deciduous tree were measured with ultrasonic anemometers. The values of the eddy diffusion coefficient during summertime have about one half of those in winter. When the density of the leaves is high, the dependency of the eddy diffusion coefficient on wind velocity is found to be very weak. The measurements imply that tree leaves reduce eddy scales by behaving as elastic obstacles.

When the fluctuating pattern of the vertical and horizontal velocities, and the temperatures at the height of 16m during summertime are analyzed as time series data, it is found that there is a dominant frequency of about 0.01 Hz in the time series. It is conceivable that the eddy-like structure whose center is positioned on the boundary of forest canopy and the open air is moving horizontally with an average velocity. The appearance of intermittent turbulent flows of sweep and ejection, which closely relate a horizontal wind velocity with a vertical one, also shows that a vertical coherent structure is formed in the canopy. In addition, the time interval between different vertical positions, indicates an eddy structure, where the flow in the lower half of the forest always precedes that in the upper half and in the open atmosphere, i.e. an elongated eddy is inclined backward and is centered on the canopy boundary.

Analytic solutions to the particle transport equations for a non-uniform atmosphere . **Robert McKibbin** (Massey University, New Zealand) IC/MT407/107

Solid and liquid particles ejected into the atmosphere by volcanic or hydrothermal eruptions, or dust and sand swept up by storms, are subsequently dispersed by atmospheric wind currents. The particles fall under gravity while being advected by the mean wind and dispersed by turbulence. Particle sizes are generally not uniform, and may change during flight, either by particle coalescence and/or fragmentation, or, in the case of fluids, by evaporation. The wind (speed, direction and dominant turbulence length scales) may also change with elevation and with time.

A quantitative model that reflects these influences on particle dispersal is outlined. The elevation-dependent features listed above are included, as well as time-dependent settling speed. In particular, analytic solutions to the advection-dispersion equations that describe the motion of the particles are found. The variation of conditions with elevation are treated by using a piecewise-constant wind velocity and dominant turbulence length scale and settling speed; this is the way that data are provided for most of the numerical schemes currently available.

Numerical results calculated directly from the derived analytical formulae are used to provide examples of the method.

IC/MP216/107: Mixing in industry and the environment.

Organiser: Jean-Luc Thiffeault (Imperial College London, UK)
Co-organiser: Emmanuel Villermaux (Université de Provence Aix-Marseille I, France)

Stirring and mixing of substances by fluid flow has been an area of active research for many decades, a reflection of its great importance for geophysical as well as industrial applications. The types of flows considered range from extremely viscous (e.g. food processing) to turbulent (e.g. combustion); from small scales (e.g. microfluidics) to large scales (e.g. atmospheric flows). Experiments have recently improved dramatically due to progress in digital optical technology. Mathematically, tools from dynamical systems, partial differential equation analysis, and stochastic analysis have been applied fruitfully to mixing problems. This minisymposium focuses on recent experiments and theory, and how these impact environmental and industrial applications.Topics addressed include:

- Measurements of stirring and mixing properties of flows;
- Optimization techniques for mixing flows;
- Measures of efficiency and diagnostics of mixing;
- Mathematical foundation of mixing:
  - The role of topological constraints;
  - Recent work on describing the concentration distribution;
  - The computation of rates of mixing.

Of particular interest is the identification of new industrial challenges for the mixing community, as well as determining which recent techniques are most promising for practical applications.

The finest scales in turbulent mixing of passive scalars. **Jörg Schumacher** (TU Ilmenau, Germany) IC/MT1183/107

The mixing of passive scalars in turbulent flows is a process with numerous applications reaching from spreading of pollutants in the stratosphere and the transport of salinity in the ocean to non-premixed combustion of fuel. Frequently, the Schmidt number which is formed as the ratio of the kinematic viscosity to the diffusivity of the passive scalar exceeds the unit value significantly. In this case, the viscous-convective range of scalar turbulence is established between the Kolmogorov dissipation scale of the flow and the Batchelor diffusion scale of the scalar. Very fine scalar filaments which are associated with strong gradients can be generated in this regime similar to chaotic advection.

The following work aims at studying the processes which cause the finest scales in turbulent mixing. We will discuss statistical and geometrical aspects of the dynamics on sub-Kolmogorov and Kolmogorov scales. As it will turn out, a continuum of local diffusion and dissipation scales is present rather than one characteristic cut-off scale. This is intimately related to the strongly intermittent nature of the dissipation rate fields for both, the passive scalar and the advecting flow.

Our investigations are based on direct pseudospectral simulations in a periodic box with large resolutions. The flow is a homogeneous isotropic turbulence which is generated by a large-scale random forcing. Scalar tubulence is sustained by an outer constant mean scalar gradient. Much effort has been put into the sufficient spectral resolution here, which significantly exceeds the usually adopted ones. This limits the range of accessible Taylor microscale Reynolds numbers on one side, but opens the opportunity for detailed studies in the far-dissipation range of the flow on the other side. Therefore, we will also present some results on the velocity statistics in the viscous range, such as statistical properties of higher order velocity gradient moments.

Chaotic mixing in industrial devices. **Emmanuelle Gouillart** (CEA Saclay, France), Olivier Dauchot (CEA Saclay, France), Stéphane Roux (Saint-Gobain, France), Jean-Luc Thiffeault (Imperial College London, UK) IC/MT2639/107

Low-Reynolds-number mixing devices are widely used in many industrial applications, such as food engineering and polymer processing. Flows are then laminar and mixing can thus be problematic without the help of turbulence. Understanding the mechanisms of laminar mixing is therefore crucial to reduce the energetic and environmental cost of mixing installations. To this respect, we know since the eighties and the introduction by Aref of the notion of *chaotic advection* [H. Aref, "Stirring by chaotic advection", J. Fluid Mech. **143**, 1984] that flows with simple time dependency can nonetheless exhibit very complicated Lagrangian dynamics due to chaos, and hence good mixing.

We report on experiments of chaotic mixing conducted in a closed vessel where a moving stirrer mixes a low-diffusivity dye with viscous fluid, and analyze quantitatively the rate at which the initial blob of dye is mixed by the flow. We find that the decay of dye concentration is slower than expected from most previous theoretical studies. The peripheral fluid region "sticking" to the vessel wall is indeed shown to slow down the whole mixing process despite exponential stretching occurring in the bulk. A minimal one-dimensional model allows us to mimic this phenomenon and yields scalings for the concentration distributions similar to the experimental observation, thus shedding light on the basic mechanisms of mixing in batch stirring devices.

Shear effects on passive scalar spectra. **Dario Vincenzi** (Max-Planck-Institut Göttingen, Germany) IC/MT2713/107

The effects of a large-scale shear on the energy spectrum of a passively advected scalar field are investigated. The shear is superimposed on a turbulent isotropic flow, yielding an Obukhov–Corrsin $k^{-5/3}$ scalar spectrum at small scales. Shear effects appear at large scales, where a different, anisotropic behaviour is observed. The scalar spectrum is shown to behave as $k^{-4/3}$ for a shear fixed in intensity and direction. For other types of shear characteristics, the slope is generally interme-

diate between the $-5/3$ Obukhov–Corrsin and the -1 Batchelor values. The physical mechanisms at the origin of this behaviour are illustrated in terms of the motion of Lagrangian particles. They provide an explanation for the scalar spectra that are shallow and dependent on the experimental conditions in shear flows at moderate Reynolds numbers.

Work done in collaboration with A. Celani, M. Cencini, E. Villermaux, M. Vergassola.

Clusters and voids of inertial particles transported by turbulence. **Massimo Cencini** (Università degli Studi di Roma "La Sapienza", Italy) IC/MT1170/107

Small impurities like dust or droplets suspended in turbulent flows are finite-size particles whose density may differ from that of the fluid and thus cannot be modeled as fluid tracers. The description of their motion, which is much more complex than that of fluid tracers, must account for their finite response time, i.e. their inertia –whence the name *inertial particles*. Remarkably such particles display strong spatial inhomogeneities even if the carrier flow is incompressible, a phenomenon known as *preferential concentration*, whose statistical description is an open issue with many industrial and environmental applications. We mention rain droplets formation and spray combustion in Diesel engines. Inertial particles are also relevant to aerosols, pollen or chemicals dispersion in the atmosphere.
Results of direct numerical simulations are presented here for inertial particles transport in homogeneous, isotropic, fully developed turbulence. The statistics of their distribution is investigated at very small scales where they form (multi)fractal objects; such clustering is very efficient for particles lighter than the fluid which transport them. At larger scales, particles do not cluster into fractal objects and different approaches are needed for understanding their statistics; here voids are the dominant structures for heavy particles. Consequences of these observations for the development of models for inertial particles transport will be also discussed.

Work done in collaboration with:
J. Bec, L. Biferale, E. Calzavarini, A. Lanotte, S. Musacchio, F. Toschi

IC/MP216/107: Mixing in industry and the environment. #2

Organiser: Jean-Luc Thiffeault (Imperial College London, UK)
Co-organiser: Emmanuel Villermaux (Université de Provence Aix-Marseille I, France)

(For abstract, see session #1 above.)

Stretching fields and lines in the transport dynamics of the Western Mediterranean. **Emilio Hernandez-Garcia** (Universitat de les Illes Balears, Spain) IC/MT2580/107

Hyperbolic points and their manifolds organize the phase space of dynamical systems. In the Lagrangian description of fluid transport they determine transport routes and mixing properties. Stretching fields are correlated with these structures and thus provide an heuristic method to approximate them. Calculations of the above mentioned objects has been performed in simplified model flows since some time ago. More recently, increased computer power and theoretical insight are allowing their identification in realistic and in observed fluid flows. In this talk I will describe recent work on the location of Lagrangian structures in velocity fields obtained from realistic simulations and from satellite altimetry of the surface layers of the Mediterranean sea. Finite Size Lyapunov exponents are found to be useful quantities to characterize stretching and compressing distributions, and their implications for mixing. Direct calculation of hyperbolic points and their stable and unstable manifolds turns out to be more complex, but allows the use of the tools of lobe dynamics to characterize fluid transport. This is illustrated here for the surface circulation in the Balearic front area.
Parts of this work have been done in collaboration with C. Lopez, V. Fernandez, F. d'Ovidio, J. Isern-Fontanet, A.M. Mancho, D. Small, and S. Wiggins.

Chaos, mixing and DNA analysis in pulsed source–sink systems. **Mark Stremler** (Virginia Tech, USA) IC/MT3053/107

DNA microarray analysis is a fluid-based, high-throughput screening technology that is helping redefine the approach to discovery in biomedical research. DNA 'target' molecules in solution are identified according to their sequence through interactions with complementary 'probe' molecules immobilized on the microarray. The standard practice of relying on diffusive 'target' transport imposes severe limitations on the speed and reliability of this technology. The logical approach is to move these molecules with an imposed flow. Efficient operation requires that the solution be well mixed and that individual molecules do not continually revisit the same area of the microarray, which suggests that chaotic transport will enhance performance. A system of pulsed source-sink pairs can produce chaotic advection in the high-aspect-ratio domains needed for microarray analysis. An analytical model of source-sink flow in a Hele-Shaw cell is used to characterize the behavior of the system as the parameters are varied, and optimal system performance is identified using standard chaos diagnostics. These analytical results are compared with an experimental analysis of mixing in a prototype system. Finally, experimental DNA hybridization results clearly demonstrate the significant signal enhancement that is produced by the presence of chaos in the system. This enhancement results in reduction of hybridization times by as much as an order of magnitude while significantly increasing the sensitivity of the test and the accuracy of the results.

Mesohyperbolicity in aperiodic flows. **Igor Mezić** (University of California, Santa Barbara, USA) IC/MT3052/107

A number of different criteria have been proposed for dynamical systems analysis of mixing in incompressible fluid flows with aperiodic time-dependence. Here we show that several of these criteria can be unified into a single finite-time criterion that depends on the Lagrangian average velocity gradient tensor. Okubo-Weiss criterion is obtained for the limit when the time interval T goes to zero, while the Lyapunov exponent criterion is obtained in the case when $T \to \infty$. Examples of controlled flows, microfluidic flows and oceanographic flows are studied.

The linked twist map approach to fluid mixing. **Rob Sturman** (University of Leeds, UK) IC/MT2867/107

Fluid mixing is a topic which spans a wide range of applications and disciplines. In recent years the tools of topological dynamical systems have been successfully employed to place the subject of chaotic mixing on a mathematical footing. In this talk we argue that the field of ergodic theory will play the next crucial role in supplying results on mixing which have a direct impact on applications.

In particular, the linked twist maps of the now classical ergodic theory literature are systems for which ergodicity, strong mixing and the Bernoulli property can be shown for sets of full measure. We show that such systems can be viewed as paradigm models for the design of fluid mixers. We give examples from diverse areas, such as microfluidics, granular flow and DNA hybridization to support this, and emphasize the key directions in which the theory could be advanced to allow a greater connection with applications.

IC/MP284/108: Influence of surfactant on interfacial flows.

Organiser: Michael Siegel (New Jersey Institute of Technology, USA)
Co-organiser: Michael Booty (New Jersey Institute of Technology, USA)

Interfacial fluid dynamics provides fertile ground for the development of analytical and numerical techniques in the study of free boundary problems. A particularly challenging class of problems arises from consideration of the effect of surfactant on the deformation and evolution of fluid interfaces. This is due to the complexity of the surfactant transport problem, which introduces coupling between surface and bulk surfactant concentrations and fluid motion, and the dependence of surface tension on surfactant concentration. Numerical computations are further complicated by the need to track highly distorted interfaces and to resolve thin boundary layers of bulk surfactant concentration. Challenges also occur in understanding how surfactants influence or may be used to control interfacial dynamics in biological and chemical applications.

The talks in this minisymposium report on recent advances in paradigmatic problems of surfactant dynamics. These include surfactant-driven instabilities in pipe and channel flows, surfactant effects on the pinch-off of bubbles and jets, and the fingering instability of a surfactant-laden droplet. The final talk presents recent results on the modeling and simulation of vesicles made of lipid bilayers, and discusses the parallels between the dynamics of vesicles and surfactant covered drops.

Surfactant-driven instability in two-fluid pipe and channel flows. **Mark Blyth** (University of East Anglia, UK) IC/MT1220/108

We consider the role of insoluble surfactant in a variety of interfacial flow phenomena. First, two-layered viscous channel flow is shown to become unstable at zero Reynolds number to a linear mode associated with the presence of surfactant. Nonlinear boundary integral calculations show that the growing wave begins to steepen and may either saturate or overturn and break. Nonlinear results at arbitrary Reynolds number computed using an immersed interface method show similar effects. The effect of both small and large wall corrugations are quantified via both linear and nonlinear calculations. Axisymmetric core annular flow in the presence of surfactant is also considered. In this case, no new instability is introduced by the surfactant; nevertheless it still has a generally destabilising influence. Nonlinear computations at arbitrary Reynolds number reveal that the surfactant plays an important role in determining the morphology of the interface, including the development of pointed waves, slugs and drops.

Spreading, dewetting and fingering in surfactant-driven thin liquid films. **Omar Matar** (Imperial College London, UK) IC/MT1367/108

The spreading of surfactant on thin liquid films is central to a number of applications including coating flow technology, surfactant replacement therapy and oil-spill cleanup. The spreading is driven by surfactant concentration gradients, which give rise to gradients in surface tension and Marangoni stresses that spread the surfactant in the direction of higher surface tension and give rise to large deformations in the thin film. Following the deposition of a droplet of surfactant solution on an initially undisturbed thin film, a thickened front is formed at the surfactant leading edge, which advances downstream of a severely thinned region, near the original point of deposition. A number of experimental studies have shown that the spreading process is accompanied by intriguing physical phenomena. Examples of such phenomena include a fingering instability that targets the thinned region. The shape of the fingers and the degree of their branching depends on the surfactant concentration and on the film thickness. Other examples involve autophobing and subsequent dewetting, which occur in situations wherein the surfactant head-group is attracted to the solid substrate underlying the liquid film through electrostatic interactions. In this talk, we present our model derived using lubrication theory which comprises a system of coupled evolution equations for the film thickness and surfactant concentration; the surfactant is allowed to exist in the bulk as a monomer and a micelle (if the concentration exceeds the critical micelle value) and on both the air-liquid and liquid-solid interfaces. Using transient growth analyses and transient numerical simulations of the two-dimensional evolution equations we demonstrate the mechanism responsible for the fingering instability. We also show results that capture the main observations in the autophobing experiments by including a disjoining pressure term in our model, which depends on the presence of surfactant and its basal adsorption.

The effect of surfactant on bubble and thread dynamics. **Michael Siegel** (New Jersey Institute of Technology, USA), Michael Booty (New Jersey Institute of Technology, USA) IC/MT3406/108

After a brief overview of the role of surfactants in the dynamics of interfacial fluid flow, we focus on two examples in the dynamics of surfactant-laden bubbles. In the first example, a surfactant-laden bubble is rapidly stretched by an imposed flow to form a dumb-bell shape, then the imposed flow is reduced to zero so that the bubble evolves solely under the action of surface tension. The usual mode of clean bubble breakup is changed by surfactant and a slender, quasisteady thread forms connecting two parent bubbles. The dynamics is elucidated by a combination of direct numerical simulation and long wave asymptotic analysis. In the second example, a surfactant-laden bubble is stretched by a steady extensional flow. Asymptotic analysis based on the slenderness of the bubble is used to find steady bubble shapes in terms of the capillary number or strain-rate of the imposed flow. At sufficiently large strain rates, a long wave analysis models the formation of experimentally observed tip-streaming filaments from the bubble end-points. In both examples, the role of effects such as small interior fluid viscosity and small diffusion of both adsorbed and dissolved surfactant is discussed.

Dynamics of surfactant-covered drops in linear flows. **Petia Vlahovska** (Dartmouth College, USA) IC/MT3425/108

Surfactants modify interfacial properties and significantly affect drop behavior in flow. I will present a systematic study of the dynamics of a drop, which is covered with a monolayer of insoluble surfactant, in linear viscous flows, both unbounded and in the presence of a wall. The effect of viscosity contrast is included. Analytical expansions for weak flows and high viscosity drops are developed. Numerical results with three-dimensional boundary integral simulations are used to explore large deformations. The results show that surfactant generally enhances drop deformation, certainly under small-deformation conditions. The steady-state drop shape and surfactant distribution are independent of viscosity contrast in straining flows (e.g. hyperbolic, axisymmetric strain). The drop shape and surfactant distribution are insensitive to viscosity contrast under small deformation conditions for any linear flow; the effect of the rotational component at higher-order. Under finite deformation conditions, the distortion of the drop shape and surfactant distribution decreases for large viscosity contrast in flows with rotation. The theory quantifies the effect of surfactant on the rheology of dilute emulsions, and predicts non-Newtonian features such as shear thinning viscosity and normal stress. I will also present calculations of the far-field hydrodynamic interactions of a surfactant-covered drops, and results about collision efficiencies and migration away from a bounding wall.

10: Fluid Mechanics, Contributed Talks

IC/CTS4829/10: **Instabilities and unsteady flows.**

Organiser: HIdeaki Aiso (Institute of Aerospace Technology, Japan)

Convective instability and optimal growth in flow over a backward-facing step. **Dwight Barkley** (University of Warwick, UK), Hugh Blackburn (CSIRO, Melbourne, Australia), Spencer Sherwin (Imperial College London, UK) IC/CT3197/102

Flow over a backward-facing step has long been a prototype for transition to turbulence in separated shear flows. Despite this, there has never been a close correspondence for this flow between what is seen in experiments and what is found in numerical stability computations. In particular, linear stability analysis has show that this flow is linearly (absolutely) stable well beyond the Reynolds numbers at which experiments show the flow to become unsteady. For some time this discrepancy has been thought to be due to the fact that the flow is convectively unstable, but previous numerical demonstrations of the convective instability of the flow have been rather qualitative.

In this talk we present result from an analysis of the optimal growth problem for the backward-facing step. We discuss how this correctly addresses the issue of convective instability of the flow. We give results from highly accurate spectral-element computations results showing pairs of optimal modes which are strongly amplified by the separated shear layer. Moreover, the evolution of these modes closely resembles what is seen in experiment.

Jeans' gravitational instability of a thermally-conducting, unbounded, partially-ionized plasma. **Aiyub Khan** (Jodhpur, India) IC/CT3898/102

The gravitational instability of an infinitely extending homogenous, partially ionized plasma, permeated by an oblique magnetic field, has been studied to investigate the effects of Hall currents, finite conductivity, viscosity, collision with neutrals and thermal conductivity on the growth rate of the disturbance. The dispersion relation obtained has been solved numerically, and it has been found that Hall currents and collision with neutrals have a destabilizing influence on the growth rate while the other mechanisms reinforce the gravitational instability. JeansŠ criterion, derived within a purely hydrodynamic framework, has been rediscussed along a nonextensive kinetic theory. A new JeansŠ criterion was deduced, which depends on the nonextensive parameter q and the standard JeansŠ wave number is recovered in the limiting case $q = 1$.

Key words: Partially Ionized; JeansŠ Criterion; Thermal Conductivity. In collaboration with Shaista Shaikh

Instabilities in buoyant flows under localized heating. **Ana Mancho** (Consejo Superior de Investigaciones Científicas, Spain), Maria Cruz Maria Cruz (Universidad de Castilla-La Mancha, Spain), Henar Herrero (Universidad de Castilla-La Mancha, Spain) IC/CT2364/107

We study, from the numerical point of view, instabilities developed in a fluid layer with a free surface, in a cylindrical container which is non-homogeneously heated from below. In particular we consider the case in which the applied heat is localized around the origin. An axisymmetric basic state appears as soon a non-zero horizontal temperature gradient is imposed. The basic state may bifurcate to different solutions depending on vertical and lateral temperature gradients and on the shape of the heating function. We find different kinds of instabilities: extended patterns growing on the whole domain which include those known as targets, and spiral waves. Spirals are present even for infinite Prandtl number. Localized structures both at the origin and at the outer part of the cylinder may appear either as Hopf or stationary bifurcations. An overview of the developed instabilities as functions of the dimensionless parameters is presented in this article.

Stability of the non-isothermal flow between co- and counter-rotating disks. **Artur Zielinski** (TU Poznan, Poland), Ewa Tuliszka-Sznitko (TU Poznan, Poland) IC/CT2380/102

The 3D DNS computations are performed to study the isothermal and not-isothermal transitional flow between two co- and counter-rotating disks enclosed by two rotating cylinders. Computations have been performed for the wide range of Reynolds numbers and different end-wall conditions including throughflow. For chosen examples 3D LES computations are performed. The investigation of the lam.-turb. transition process inside the inter-disk 3D rotating flow is of great interest for the internal aerodynamics of engines. The flow is described by 3D Navier-Stokes, energy and continuity equations. To take into account the buoyancy effects induced by the involved body forces the Boussinesq approximation is invoked. Numerical computations are based on a pseudo-spectral Chebyshev-Fourier method. The time scheme is semi-implicit and second-order accurate [1]. For LES computations, a Lagrangian dynamic sub-grid model of turbulence is used, [2]. In this paper we studied the spatial structures which appeared in different stages of the lam.-turb. transition process. We considered cavities of the aspect ratio ranging from 9 to 11 and curvature parameters Rm=1.5Ů3.0. For sufficiently large negative value of the rotational rate of disks we observed the instability pattern which corresponds to the negative spirals described in [3]. We investigated influence of the thermal Rossby number on lam.-turb. transition process. Distributions of the local Nusselt numbers obtained on the heated rotating disk showed good agreement with the experimental results. For chosen examples, DNS and LES results are compared.

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Numerical instability of shock waves in conservative difference approximation of the compressible Euler equations. **HIdeaki Aiso** (Institute of Aerospace Technology, Japan) IC/CT3013/106

It is known that some instability may happen along with shock waves in numerical computation for the compressible Euler equations. Even with the discretization by Godunov scheme, which is considered one of the most natural discretization, such instability may happen.
Mentioned by Quirk in 1994, the instability of numerical carbuncle phenomenon has been discussed in several articles. The instability may happen in multi-dimensional computation but not in one dimensional computation, and usually destroys the numerical computation. On the other hand the linear instability of one dimensional shock profile has been also discussed. But this kind of instability does not seem to cause any fatal error while it does harm with the numerical convergence to some expected stable state. The relation between two kinds of instability phenomena above is not enough analyzed.
We observe the linear stability of numerical computation of fixed and progressing shock waves using Godunov scheme in one and multi- dimensional cases by observing the linearized system of all of the calculated variables in the computation. The method of analysis is first proposed by Moschetta et al. We extended the analysis to the case of progressing shock waves and obtain the following results. (1)In cases of completely upwind computation of progressing shock wave, the occurrence of carbuncle phenomenon and the linear instability of multi-dimensional numerical system show rather exact coincidence. It means that the carbuncle instability is caused by the linear instability in the cases. (2)In cases of fixed shock wave the occurrence of carbuncle and the linear instability shows some coincidence but it is not exact. Some relation with linear instability of one dimensional shock profile is also observed.

Slowly moving shock cases also show some critical situation. We also discuss the multi-dimensionality of carbuncle phenomenon from the numerical experiments.

Octopus-shaped instabilities of evaporating droplets. **Nebojsa Murisic** (New Jersey Institute of Technology, USA), Lou Kondic (New Jersey Institute of Technology, USA) IC/CT782/108

We report on curious phenomena recorded recently during spreading of evaporating isopropyl alcohol droplets on silicon wafer surfaces (for movies, see http://m.njit.edu/~kondic/thin_films/octopi.html). Novel *octopus*-shaped instabilities were noticed appearing close to the contact line. In addition to our desire to understand the instability, a motivation for this study is the fact that instabilities occurring in evaporating droplets are the signature of rich dynamics which influences drying, dewetting, and even solid residue deposition which can deteriorate electrical and other properties of the semiconductor devices.
After discussing the experimental results, we present a lubrication-based mathematical model describing spreading of volatile drops on non-isothermal solid substrates. We show that evaporation is not limited by diffusion of vapor into surrounding gas phase, and therefore utilize the one-sided model, where the problem is to be solved for liquid only. The starting point in the model development are Navier–Stokes equations in 2D for incompressible viscous fluid, accompanied by the energy equations for liquid and solid phase, and appropriate boundary conditions. Application of lubrication approximation yields a single nonlinear PDE for evolution of drop thickness. We employ finite-difference-based numerical algorithm to simulate drop evolution and perform linear stability analysis (LSA) of the full governing equation. Through LSA and numerical simulations, we show that essential factors influencing occurrence of octopus-shaped instabilities include volatility of liquid, and thermal conductivity of both liquid and solid.

The presented theoretical work was done in collaboration with the experimental work by Dr. Y. Gotkis (KLA Tencor) and Dr. I. Ivanov (Blue29).

IC/CTS4933/10: Free surface, flow, fluid–structure stratified.

Organiser: Daniel Anderson (George Mason University, USA)

Approximate factorization methods for free-surface flows. **Cassio Oishi** (Universidade de São Paulo, Brazil) IC/CT846/101

When solving the unsteady incompressible Navier–Stokes equations the velocity and pressure fields are coupled, giving rise to a large system equations. Such systems can be difficult to solve, not just because of their nonlinearity, but their very size can make the problem intractable. To overcome this difficulty one approach is to apply a projection method to decouple the Navier-Stokes equations. In the context of the Marker-And-Cells method [F.H. Harlow and J.E. Welch, Physics of Fluids, 8 (1965) 2182-2189], which is one of the first techniques for successfully solving free surface flow problems, this work investigate the order of accuracy of projection methods when applied to free surfaces flows. This investigation is carried through the method of approximate factorization (introduced initially for Navier-Stokes equation by [J.K. Dukowicz and A. S. Dvinsky, Journal of Computational Physics, 102 (1992) 336-347]). In this work we shall show that it is possible to apply the method of approximation factorization to derive a strategy for obtaining a second-order projection method for free surface flows. It will be noted that the order of the method is not influenced by how one updates the pressure and the boundary conditions. This will emerge naturally from an analysis of the error term. Numerical results illustrating the different performances of the two approaches will be presented for a 2D free surface flow problem. Examples of the second-order projection method for 3D free surface problems will also be presented.

Work done in collaboration with Jose A. Cuminato and Valdemir G. Ferreira

Homogenization theory for nonlinear free-boundary problems. **Daniel Anderson** (George Mason University, USA) IC/CT2068/100

We explore homogenization theory applied to nonlinear free-boundary problems. Problems under consideration include simple one-dimensional problems such as the draining of a horizontally-layered porous material, slender two-dimensional gravity currents slumping in a heterogeneous porous media, and fully two-dimensional gravity currents. The description we consider uses a sharp moving interface to define the fluid region in each case. We discuss details of how these problems can be homogenized with respect to rapidly-varying permeability fields to obtain effective, leading-order, descriptions of each flow. Of particular interest is the possibility of identifying corrections to the leading-order homogenization results. Such corrections lead to approximate solutions that incorporate more completely the physical features of the problem associated with the rapid variations.

Numerical techniques for ice-mass dynamics simulation by using a complete shallow ice approximation. **Carlos Vázquez Cendón** (Universidade da Coruña, Spain), Natividad Calvo-Ruibal (Universidade de Vigo, Spain), José Durany (Universidad de Vigo, Spain), Raquel Toja (Dep. Mathematics, Faciulty of Informatics, Campus, Spain) IC/CT2140/103

In this work a complex coupled shallow ice model governing thermal, hydrodynamic and mechanical processes in large ice masses dynamics is proposed and solved by means of efficient numerical techniques. For this, the PDE system governing the upper ice sheet profile (1), the velocity field, the temperature and the basal magnitudes is posed and a fixed point iteration which sequentially treats each subproblem is developed (2). In addition to the the nonlinear equations, free/moving boundary problem formulation for unknown domains are required. Several numerical techniques have been considered: 1-d and 2-d first order characteristics methods for time discretization, 1-d and 2-d finite elemens for spatial discretization, duality and Newton methods for nonlinear problems, numerical quadrature formulas for velocity computation, etc. (2). For the numerical simulation a software toolbox application has been developed (3). Furthermore, in order to save computing time in real applications, appropriate parallel implementations of BICGSTAB linear systems solver combined with mean grain parallel techniques have been applied (4).

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Numerical modelling of fluid-structure interaction with application in hemodynamics. **Anna Zauskova** (TU Hamburg–Harburg, Germany), Mária Lukáčová (Hamburg University of Technology, Germany) IC/CT1270/105

The aim of this work is the numerical approximation of the blood flow in compliant vessels. In this mathematical model we consider blood as a non-Newtonian fluid in a domain, which is deformed by acting of the fluid forces. In this fluid-structure interaction problem, the Navier-Stokes equations with non-linear stress tensor for the fluid are coupled with the domain deformation equation governing on the deforming part of the boundary. A global iterative method with respect to the domain deformation is used to decouple the fluid and structure. Some numerical experimets are presented and the convergence of the global iterative method can be observed. We will also present theoretical analysis of the mathematical model for shear dependent non-Newtonian fluids in compliant vessels.

Corner singularities of compressible Navier–Stokes equations on polygonal domains. **Jae Ryong Kweon** (Pohang Univ. of Science and Technology, Republic of Korea) IC/CT4316/104

In this talk I will discuss the compressible Navier–Stokes equations on polygonal domains. The solution velocity is split into singular plus regular parts near concave corners. The stress intensity factor is a function of time variable, has certain regularity. By a formula of pressure we observe propagation of corner singularity along the streamlines emanating from the corners and unboundedness of derivatives of pressure there. An increased regularity for the remainder is obtained.

Complete analysis of an ideal rotating uniformly-stratified system of ODEs. **Bhausaheb Desale** (University of Mumbai, India) IC/CT2611/101

In this paper we discuss a system of six coupled ODEs which arise in ODE reduction of the PDEs governing the motion of uniformly stratified fluid contained in rectangular basin of dimension $L \times L \times H$, which is temperature stratified with fixed zeroth order moments of mass and heat. We prove that this autonomous system of ODEs is completely integrable if Rayleigh number $Ra = 0$ and determine the stable, unstable and center manifold passing through the rest point and discuss the qualitative feature of the solutions of this system of ODEs.

This work is done in collaboration with Professor G. K. Srinivasan

IC/CTS4824/10: Mathematical theory.

Organiser: Hyeong-Ohk Bae (Ajou University, Republic of Korea)

Regularity for the Navier–Stokes equations with slip boundary condition. **Hyeong-Ohk Bae** (Ajou University, Republic of Korea) IC/CT2911/103

For the Navier–Stokes equations with slip boundary conditions, we obtain the pressure in terms of the velocity. Based on the representation, we consider the relationship in the sense of regularity between the Navier-Stokes equations in the whole space and those in the half space with slip boundary data.

Group-invariant solution for a free 2D turbulent jet with eddy viscosity. **David Mason** (University of the Witwatersrand, South Africa), Des Hill (University of Western Australia) IC/CT3690/108

A free two-dimensional turbulent jet described by eddy viscosity is analysed. A Lie point symmetry generator of the two-dimensional boundary layer equations for the turbulent jet exists provided the eddy viscosity satisfies a first order quasi-linear partial differential equation. The general form of the group invariant solution for the fluid velocity and the eddy viscosity is derived. The hypothesis due to Prandtl that the eddy viscosity is constant across a turbulent jet is investigated. Using the group invariant solution a numerical solution is derived in which the eddy viscosity varies across the jet. The results are compared with the corresponding results for a laminar two-dimensional jet.

On nonlinear and linear instability of the Rossby–Haurwitz wave. **Yuri Skiba** (Universidad Nacional Autónoma de M'exico, Mexico) IC/CT592/102

The stability of meteorologically important Rossby–Haurwitz (RH) waves in an ideal incompressible fluid on a rotating sphere is studied. A RH wave of degree n is the sum of a super-rotation flow of H_1 and a polynomial of H_n (H_k is the subspace of homogeneous spherical polynomials of degree k). By a conservation law derived for perturbations, perturbation energy $E(t)$ and enstrophy $\eta(t)$ decrease, remain constant or increase simultaneously. This divides all the perturbations into invariant sets M_-, M_+ and M_0 where $\chi(t) - n(n+1)$ is negative, positive or zero, respectively, and $\chi(t) = \eta(t)/E(t)$ is the perturbation spectral number. Also, M_0 is divided in invariant sets H_n and $M_0 - H_n$. Subspace H_n of neutral perturbations is used as the zero class to introduce a factor space and factor norm of perturbations. The sum of the energy and factor norms is a good norm in the instability study, since the energy norm controls the perturbation part of H_n, and the factor norm -

the perturbation part orthogonal to H_n. It is shown that any RH wave of H_1 is Liapunov, and hence, linearly stable, while any non-zonal RH wave of $H_1 + H_n$ where $n > 1$ is Liapunov unstable to perturbations of M_-. The instability mechanism has nothing in common with Poincare instability being identical with that of a periodic solution to nonlinear pendulum. It is proved that $\chi(t) = n(n+1)$ is the necessary condition for exponential instability (an unstable mode belongs to $M_0 - H_n$). The maximum growth rate of unstable modes is estimated, and the orthogonality of an unstable mode to the RH wave is shown both in the inner product of square integrable functions and in the energy inner product.

Generalized analytic functions in 3D Stokes flows. **Michael Zabarankin** (Stevens Institute of Technology, USA) IC/CT4463/103

A class of generalized analytic functions, defined by a special case of the Carleman system that arises in 3D asymmetric problems of hydrodynamics of Stokes flows, stationary electromagnetic fields in conductive materials, etc., has been considered. Hilbert formulas, establishing relationships between the real and imaginary parts of a generalized analytic function from this class, have been derived for the domains exterior to the contour of spindle, lens, bi-spheres and torus in the meridional cross-section plane. This special case of the Carleman system has been reduced to a second-order difference equation with respect to either the coefficients in series or densities in integral representations of the real and imaginary parts. For spindle and lens, the equation has been solved in the framework of Riemann boundary-value problems in the class of meromorphic functions. For torus, the equation has been solved by means of the Fourier transform, while for bi-spheres, it has been solved by an algebraic method. As examples, analytical expressions for the pressure in the problems of the 3D axially symmetric Stokes flows about rigid spindle-shaped body, lens-shaped body, bi-spheres and torus have been derived based on the corresponding Hilbert formulas.

Non-degeneracy, from the prospect of wave–wave regular interactions of a gas-dynamic type. **Liviu Florin Dinu** (Institute of Mathematics of the Romanian Academy), Marina Ileana Dinu (Polytechnical University of Bucharest, Romania) IC/CT2483/104

An analogue of the genuinely nonlinear character of a one-dimensional simple wave solution is identified and essentially used in the construction of some multidimensional extensions (simple waves solutions, regular interactions of simple waves solutions). A class of exact multidimensional gasdynamic solutions is constructed whose interactive elements are regular.
A *parallel* is constructed between Burnat's algebraic approach (which uses a *dual* connection between the hodograph and physical characteristic details) and Martin's differential approach (centered on a Monge-Ampère type representation) regarding their contribution to describing some nondegenerate gas-dynamic (one-dimensional, multi-dimensional) regular interaction solutions. Some specific aspects of the multidimensional algebraic description are beforehand identified and classified with an admissibility criterion selecting a *genuinely nonlinear* type where other (hybrid) types are formally possible.

IC/CTS4825/10: Aerodynamics and MHD.

Organiser: Purna Kaloni (University of Windsor, Canada)

Influence of double stratification on MHD free convection with Soret and Dufour effects in a Darcian porous media. **Shyam Tak** (Jai Narain Vyas University, India) IC/CT3907/100

Abstract
The heat and mass transfer characteristics of natural convection about a vertical surface embedded in a doubly stratified saturated porous medium subjected to a magnetic field is studied, taking into account the Dufour and Soret effects. It is found that the similarity solution exists for the case of uniform surface heat and mass flux conditions when the thermal and solutal stratification of the medium are assumed to have power function of x. The resulting set of ordinary coupled nonlinear differential equations is solved numerically using shooting technique. Dimensionless velocity, temperature and concentration profiles are presented graphically and Nusselt and Sherwood numbers are tabulated for various values of the involved parameters. It is observed that the velocity, temperature and concentration profiles for thermal and solutal stratified ambient fluid- porous medium are, in general, smaller than those for the isothermal and iso-solutal ambient fluid-porous medium.

Keywords: Natural Convection, Double Diffusion, Double stratification, Magnetic Field, Darcian porous media. In collaboration with Arti Lodha

Convection problems in magnetic fluids. **Purna Kaloni** (University of Windsor, Canada) IC/CT3423/107

Magnetic fluids are colloidal suspensions of ferromagnetic nano particles in a nonmagnetic carrier fluid.Each particle has a permanent magnetic dipole moment 'm' but due to thermal agitation the suspension has no net magnetization in the absence of an external field.Depending upon the size of the particles,their concentration and the consideration of rotation,a variety of equations have been proposed to describe them. Convective stability problems under a constant magnetic field or a time periodic field in the simpler theories have already been discussed in the literature, with interesting results. Our purpose here is to study these problems in a most general theory,and in both kinds of magnetic fields.

A new stretch–twist–fold model for fast dynamo. **Renzo Ricca** (Università degli Studi di Milano Bicocca, Italy), Francesca Maggioni (Università degli Studi di Milano Bicocca, Italy) IC/CT3142/103

New equations for the Stretch-Twist-Fold (STF) cycle, originally proposed by Vainshtein and Zeldovich (1972) for the generation of fast dynamo of magnetic fields, are presented and applied to a magnetic flux-tube with twist, following Ricca (*Fluid Dyn. Res.* **36**, 2005). Analytical minimization of the magnetic energy functional is made by using curvilinear, orthogonal coordinates and under the mild constraint of circular tube cross-section and uniform twist field distribution. We show that under appropriate kinematics the constrained minimized energy can grow super-exponentially in time, without necessarily involving high twist rates, hence providing a lower bound on the growth of magnetic energy of the system. These results shed new light on possible efficient mechanisms of magnetic field generation and sustainment for astrophysical and laboratory plasmas.

MHD stagnation-point flow of a non-Newtonian fluid . **Fotini Labropulu** (Luther College-University of Regina, Canada) IC/CT2568/103

The unsteady two-dimensional stagnation point flow of the Walters B' fluid impinging on an infinite plate in the presence of a transverse magnetic field is examined and solutions are obtained. It is assumed that the infinite plate at $y = 0$ is making harmonic oscillations in its own plane. A finite difference technique is employed and solutions for small and large frequencies of the oscillations are obtained for various values of the Hartman's number and the Weissenberg number.

Numerical simulation of Darrieus and Savonius wind-turbine aerodynamics. **Dmytro Redchyts** (National Academy of Sciences of Ukraine, Kyiv), Andrei Zinchenko (Dniepropetrovsk, Ukraine), Olexander Prykhodko (Prykhodko, Ukraine) IC/CT4407/103

The report covers the typical aspects of numerical simulating dynamics and aerodynamics of vertical-axis wind turbines, such as selection of initial mathematical model and the model of turbulence, selection of the numerical method, verification of initial mathematical model and testing of the numerical method, post-processing and visualization of results obtained. Presented method is based on the joint solution of the wind turbine rotation equations and the equations for non-stationary incident wind flow. Simultaneous solution of the aerodynamics equations and the equation of rotor spinning relative to fixed axis under the action of the incident airflow and the fixed loading gives the current rotation speed of wind turbine. The algorithm based unsteady Reynolds averaged Navier-Stokes equations (RANS) used for calculation of aerodynamic characteristics. To close the governing equations following turbulence models were used: SA, SARC and SALSA. Solution of governing equations is obtained using the implicit finite-volume numerical algorithms based on artificial compressibility method and multi-block overlapped structured grids. Verification of the CFD algorithms and codes developed is carried out applying the problems on flow in a cavity and around the fixed and rotating cylinders. Comparison of the turbulence models is given for a flow around the NACA 4412 airfoil. Instantaneous streamlines, vorticity fields and hysteresis of the unsteady aerodynamic characteristics are discussed for an oscillating NACA 0015 airfoil. It is shown that SALSA model demonstrates its advantages on massive flow separation and dynamic stall. Results for Darrieus and Savonius rotors with different geometrical characteristics and different number of blades are presented. Physical features of the flow near wind turbine blades, such as boundary layer separation and flow interactions between the blades, are discussed.

A contractive operator solution of an airfoil design inverse problem. **Jan Šimák** (Aeronautical Research and Test Institute, Czech Republic), Jaroslav Pelant (Aeronautical Research and Test Institute, Czech Republic) IC/CT4297/106

This paper deals with a numerical method for an airfoil design[1]. The method is intended for design of an airfoil from a given velocity distribution along a mean camber line. The stagnation point has to be in the beginning of the mean camber line. The method is based on searching for a fixed point of a contractive operator. This operator combines an inexact inverse operator and equations describing the flow. We assume a subsonic flow described by a system of Euler equations which is solved by an implicit finite volume method. Newton method is applied to the solution of the nonlinear system. The resulting system of linear algebraic equations is solved by GMRES method, the Jacobian-free version is described. The inexact inverse operator constructs a middle curve function and a thickness function with respect to the given velocity distribution. In addition to the velocity distribution the velocity in infinity is given. The angle of attack is determined so that the stagnation point is in a specific position. Successful numerical results are presented.

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IC/CTS4827/10: Multi-phase flow and free surfaces.

Organiser: Gerald Kleinstein (Northeastern University, USA)
Co-organiser: Bronislav Librovich (University of Strathclyde, UK)

Non-equilibrium gas–liquid transition model. **Bronislav Librovich** (University of Strathclyde, UK), Andrew Nowakowski (University of Sheffield, UK), Savvas Tassou (Brunel University, UK), Issa Chaer (Brunel University, UK) IC/CT3047/107

A new rigorous mathematical model for evaporation/condensation, including boiling, has been proposed. A problem of phase transition and in particular evaporation/condensation is one of the most acute problems of modern technology with numerous applications in industry, such as: in refrigeration, distillation in chemical industry. It is very common to use equilibrium evaporation model, which assumes that concentrations of species in the gas phase is always at saturated condition. Such kind of approach can lead to significant errors, resulting in negative concentrations in complex computer simulations. In this work two analytical solution of simplified differential-algebraic system have been obtained. One of them was deduced using assumption that the process is isothermal and gas volume fraction is constant. In the second solution the assumption about gas volume fraction has been removed. The code for numerical solution of differential-algebraic system, using conservative scheme, has been developed. It was designed to solve both systems of equations with boiling and without. Numerical calculations of ammonia-water system with various initial conditions, which correspond to evaporation and/or condensation of both components, have been performed. It has been shown that, although system quickly evolves to quasi equilibrium state (the differences between current and equilibrium concentrations are small) it is necessary to use non-equilibrium evaporation model, to calculate accurately evaporation/condensation rates, and consequently all other dependent variables.

Application of high-performance solvers for multiphase flow calculations. **Andrei Zinchenko** (Dniepropetrovsk, Ukraine) IC/CT4126/106

Calculations of heat and mass transfer in heterogeneous media require significant computational efforts in comparison with similar single-phase flows. From the other hand numerical algorithms for such problems are suitable for effective parallelization includes two stages. First of all each phase could be computed separately within one iteration due to explicit form of gas-particle interaction terms. Also we can use the parallelization techniques developed for single-phase flows when computing each phase.

Basing on these ideas the parallelization techniques such as multigrid algorithms, high order difference schemes using flux vector splitting, tracer methods for discrete phase were implemented in applied program package. Well-known and author's developed difference schemes implementation such as TVD-like and compact high order discretizations on the structured block grids were developed.

The problem of interaction of shock waves with gas-particle boundary layer on curvilinear profiles was solved on cluster of personal computers connected with Fast Ethernet network. The particles volume fraction and diameter influence to the

flow separation in interaction zone was investigated. The impact of heating and cooling the surface on boundary layer flow was computed also. Calculation shows above linear acceleration of calculating speed for large scale grids.

Implementing algorithms in the integrated program packages simplifies developing and testing new methods and schemes in both sequential and parallel versions.

The evolution of a viscous two-fluid flow down an inclined plane. **Jürgen Socolowsky** (FH Brandenburg, Germany) IC/CT3940/101

A model describing the unsteady motion of two viscous incompressible fluids down an inclined plane is considered. Both fluids are flowing jointly. At their contact surface and at the free surface we are given the usual free boundary conditions. Thus, the mathematical model represents a non-stationary free boundary value problem for the Navier-Stokes equations. The problem is two-dimensional and it describes the flow regime on some part of different coating devices in Mechanical Engineering. The complete problem is linearized over the steady-state solution. For small initial perturbations the existence of a unique solution, local in time, to the full problem can be shown.

Free-surface film flow over topography under electric fields. **Dmitri Tseluiko** (University of East Anglia, UK) IC/CT4372/101

We investigate a two-dimensional gravity-driven flow of a perfectly conducting viscous liquid down an inclined topographical feature in the presence of a normal electric field. Our interest lies in predicting the free-surface shape of the liquid, particularly the dependence of it on an electric field. Long-wave asymptotic analysis is used to derive a non-linear evolution equation for the interface. We analyse steady-state solutions for flows into a trench and over a mound of a very wide aspect ratio. The sharp-edged walls are approximated by hyperbolic tangent functions and the dependence of the solutions on the parameter that controls the steepness of the walls is analysed. In the absence of an electric field the solution develops a capillary ridge above a downward step and a slight depression in front of an upward step. It is shown that increasing the electric field can completely eliminate the capillary ridge whilst introducing a slight depression right after the downward step, and the film is pulled away from the step. For upward steps the behaviour is opposite Ű the depression in front of an upward step can be completely eliminated by an electric field, while a slight ridge is formed right above the step, and the film is pulled towards the step. The results are corroborated by fully non-linear boundary integral calculations for Stokes flow. The work was done in colloboration with M. Blyth, J.-M. Vanden-Broeck, D. T. Papageorgiou.

Impulsive displacement of liquid in a pipe. **Gerald Kleinstein** (Northeastern University, USA) IC/CT4411/103

We consider the motion of a liquid, originally at rest in a long circular pipe, which is being displaced by another liquid. The purpose of this paper is to show that the displacement problem can be solved by an inviscid analysis, and to establish the displacement time; the time it takes to completely displace the liquid originally at rest in the pipe. As shown by Kleinstein (1988), under impulsive conditions an irrotational initial state may exist but cannot persist; the irrotational motion of the fluid must transition into a viscous motion consistent with the second law of thermodynamics. It is anticipated that in the present problem, due to its impulsive nature, an essentially "inviscid window" may exist for the initial motion. Assuming the time scale of the liquid displacement problem falls primarily within this inviscid window, the solution of the problem could proceed by an inviscid analysis. To test this hypothesis we consider the model of a liquid displaced by the same liquid for which an exact solution of the Navier-Stokes equations exists. Analyzing this model we obtain that the displacement time is essentially inviscid with a small viscous correction of the order of $(l/d)R_p^{-1}$ where R_p is a Reynolds number based on the pressure difference, and l/d is the ratio of length to diameter of the pipe. As additional support for the application of an inviscid analysis to the two liquid problem we show that at the displacement time the viscous layer next to the wall is very thin, it is also of the order of $(l/d)R_p^{-1}$, that the velocity profile, with the exception of the sharp drop near the wall to satisfy the no-slip condition, is essentially flat; and, that the liquid-liquid interface consists of a cylindrical shell, anchored at the ring $x(a,0)=0$, which makes a steep angle with the wall, and at $x=l$ it is cut by essentially a flat surface. We accept these results from the single liquid model, together with the assumption that the viscous correction remains essentially of the same order, as justification for the application of an inviscid analysis to the two liquid problem. Using a control volume analysis, we obtain two coupled ordinary differential equations for the motion of the interface. Combining these two equations results in a single non-linear ordinarry differential equation for the position of the interface for which a closed form solution is derived. We show that the lower the density of the displacing liquid as compared with the density of the displaced liquid, the shorter the displacement time is. In particular, for a horizontal pipe, at the limit when the ratio ρ_A/ρ_B approaches zero, we obtain an explicit expression for the displacement time in the formula, $t_D = l\{(\pi/2)[\rho_B/(p_A-p_B)]\}^{1/2}$ as compared with $t_D = l[2\rho/(p_A-p_B)]^{1/2}$ for the case when $\rho_A=\rho_B$.

Breakup of finite fluid films. **Lou Kondic** (New Jersey Institute of Technology, USA), Javier Diez (UNICEN de Buenos Aires, Argentina) IC/CT4508/108

We study the breakup process of thin fluid films that partially wet a solid surface. Using long-wave (lubrication) approximation, we formulate a nonlinear partial differential equation governing the evolution of the film thickness. This equation includes the effects of capillarity, gravity, and additional conjoining/disjoining pressure term to account for intermolecular forces. We perform standard linear stability analysis of an infinite flat film, and identify the corresponding stable, unstable and metastable regions. Within this framework, we analyze the evolution of a semi-infinite film. The numerical simulations show that for long and thin films, the dewetting fronts of the film generate a pearling process involving successive formation of ridges at the film ends and consecutive pinch-off behind these ridges. On the other hand, for shorter and thicker films, the evolution ends up by forming a single drop. The time evolution as well as the final drops pattern shows a competition between the dewetting mechanisms caused by nucleation and by free surface instability. We find that precise computations, requiring quadrupole precision of computer arithmetic, are often needed to avoid spurious results.

IC/CTS4826/10: Turbulence and transition.

Organiser: Nikolai Kornev (Universität Rostock, Germany)

Turbulent–laminar patterns in plane Couette flow. **Laurette Tuckerman** (LIMSI, France), Dwight Barkley (University of Warwick, UK) IC/CT3187/102

Recent experiments by Prigent and Dauchot have shown that the remarkable spiral turbulence state of Taylor-Couette flow also occurs in plane Couette flow. In both cases, a pattern of alternating turbulent and laminar bands appears at a well-defined Reynolds number. The pattern is tilted with respect to the streamwise (or azimuthal) direction and its wavelength is much larger than the gap; the angle and wavelength depend systematically on Reynolds number. We have numerically simulated these turbulent-laminar patterns for plane Couette flow. In our computational approach, we replace the very large lateral dimensions of the experiment by a narrow and periodically repeating rectangle which is tilted with respect to the streamwise direction. In this way we determine which angles and lengths support turbulent bands. Our computations show a rich variety of turbulent-laminar patterns as the angle and Reynolds number are varied, including spatio-temporal intermittency, branching and travelling states, and localized states analogous to spots. A quantitative analysis of the mean flow of a regular turbulent-laminar pattern reveals that the flow in the quasi-laminar region represents a non-trivial balance between the viscous and advective forces (unlike ordinary laminar Couette flow, in which both forces are zero). Surprisingly, the mean flow and turbulent forces over the entire domain is exactly centro-symmetric and consists of only three trigonometric functions.

Synthesis of artificial turbulent fields with prescribed second-order statistics using the random-spot method. **Nikolai Kornev** (Universität Rostock, Germany), Hannes Kröger (Universität Rostock, Germany), Egon Hassel (Universität Rostock, Germany) IC/CT3362/106

The synthesis of artificial turbulent fields with prescribed statistical properties is an important problem for specification of inlet conditions in LES and DNS simulations.

The starting point of our novel method is the concept of a turbulent flow as a motion of turbulent spots arising at random positions at random times. Each random spot has an inner distribution of velocity which is found from the condition that the statistical properties of the artificial turbulent field are equal to the prescribed ones. In the case of a homogeneous turbulent field we found an analytical solution for the inner distribution provided the autocorrelation functions $\rho(\eta,0,0)$, $\rho(0,\eta,0)$ and $\rho(0,0,\eta)$ (or the corresponding one dimensional energy spectra) and r.m.s of fluctuations are known. In the case of inhomogeneous turbulent fields the solution can be obtained from numerical solution of an integral equation derived from the definition of the correlation function (see Kornev, N. and Hassel, E., 2006, Method of random spots for generation of synthetic turbulent fields with prescribed autocorrelation functions, Commun. Numer. Meth. in Engng, **DOI**:10.1002/cnm.880.).

The field of velocity fluctuations is then conditioned and transformed so that the one-point cross correlations between different velocity components (Reynolds stresses) are taken into account. We propose the transformation which allows to take the Reynolds stresses into acount and doesn't disturb the two-point statistics. A simplified version of the method is developed to generate the velocity field with prescribed integral lengths.

The method is implemented in the software package OpenFoam and used for LES and DNS simulations. The method allows to generate velocity fields with prescribed spatial integral length scales, integral time scales, two-point spatial and one point temporal autocorrelations, as well as one-point cross correlations between fluctuation components. The method has two important advantages in comparison with the other methods capable to generate fields with prescribed two-point statistics. They are the grid independency and simple analytical solutions for the homogeneous case.

Using divergence-free and curl-free wavelets for the simulation of turbulent flows. **Valérie Perrier** (Université Grenoble I, France) IC/CT4086/106

The prediction of fully-developed turbulent flows represents an extremely challenging field of research in scientific computing. The *Direct Numerical Simulation* (DNS) of turbulence requires the integration in time of the full nonlinear Navier–Stokes equations; that is, the computation of all scales of motion.

In that context, wavelet bases provide a decomposition of the solution allowing to represent the intermittent spatial structure of turbulent flows with only few degrees of freedom. For incompressible flows and the Stokes problem, an interesting approach first considered by K. Urban[5], was to use the *divergence-free wavelet bases* originally designed by P.G. Lemarié-Rieusset[4].

In the present talk, we investigate the use of divergence-free wavelets for the simulation of turbulent flows. First we present the divergence-free and curl-free vector wavelets, with their algorithmic implementations in 2D and 3D, leading to fast algorithms (in $\mathrm{O}(N)$ operations where N is the number of grid points)[3]. Then we define an iterative procedure to compute the Helmholtz decomposition of any compressible field, in a wavelet formulation[2]. These ingredients allow us to derive a numerical method for the Navier–Stokes equations, based on divergence-free wavelets. Finally we present numerical tests in 2D to validate the approach[1].

This is work done in collaboration with E. Deriaz.

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The multi-spectral decimation scheme for turbulence simulations. **Malcolm Roberts** (University of Alberta, Canada), John Bowman (University of Alberta, Canada) IC/CT3201/106

Shell models of the Gledzer–Ohkitani–Yamada (GOY) type can provide an excellent testbed for new ideas and methods for two- and three-dimensional turbulence. We review some results for Navier–Stokes turbulence and compare with results for shell models. We introduce a *multi-spectral* decimation scheme for high-Reynolds number turbulence simulations.

The nonlinear coupling coefficients on the coarse grid are calculated with a modification of the method of spectral reduction [Bowman, Shadwick, and Morrison, *Phys. Rev. Lett.* **83**, 5491 (1999)]. This decimation scheme exploits the continuity of moments of the underlying probability distribution function to replace neighbouring shells by a reduced number of representative shells with enhanced couplings. The projection and prolongation operators between the grids are designed to conserve energy.

We demonstrate how this multi-spectral scheme might be used to derive a reliable dynamic subgrid model for turbulence.

Regular reflection up to the transition point. **Volker Elling** (Brown University, USA) IC/CT4434/104

Reflection of a weak shock from a solid wedge is a classical problem in gas dynamics studied by Ernst Mach and John von Neumann. There are several possible flow patterns, depending on parameters like wedge sharpness and shock strength. For sufficiently blunt wedges, *regular reflection*, the qualitatively simplest pattern, is observed; as the wedge becomes sharper either *simple*, *double* or *complex Mach reflection* emerge. It is not clear when the transition between regular and Mach reflections occurs. Several criteria have been proposed; it has has even been suggested that there may be bistable flows where regular and Mach reflection are both possible and a change of type can arise from a perturbation. Experimental and numerical evidence is not quite conclusive because physical and numerical boundary layers and other phenomena can blur the picture; for example they can generate spurious Mach stems in a case where regular reflection is observed in perfectly inviscid flow.

Recently, Chen and Feldman have succeeded in constructing regular reflection as an *exact* solution, for compressible potential flow with wedge angle close to $180°$. Elling and Liu independently found different techniques of constructing exact solutions of potential flow and applied it to the classical problem of weak vs. strong shock waves in supersonic flow onto wedges.

In the present work we adapt the techniques of Elling and Liu to show that they are capable of solving regular reflection as well. We demonstrate that the *sonic criterion* is the correct criterion for transition from regular to Mach reflection. For some upstream Mach numbers and sufficiently large γ, including the important $\gamma = 5/3$, we construct exact solutions up to the transition point.

Turbulence simulation using rapid distortion theory. **Mosa Chaisi** (National University of Lesotho) IC/CT4805/106

A fairly simple method of simulating a turbulent domain of a fluid body is demonstrated; which is also fairly inexpensive in terms of computing resources needed to carry it out. The underlying theory employed in dealing with the Navier-Stokes (N-S) equations is what is referred to as Rapid Distortion Theory - linearised N-S equations. Amongst the many physical scenarios where this can be useful, momentum exchange across a gas-liquid interfaces, turbulent mixing and surface renewal are explored with the help of flow visualization in the form of vector plots, flow animation and particle tracking techniques.

IC/CTS4828/10: Numerical schemes and algorithms.

Organiser: Robert Krasny (University of Michigan, Ann Arbor, USA)

A mesh adaptation for non-stationary problems. **Jiří Felcman** (Univerzita Karlova, Czech Republic), Petr Kubera (Purkyne University, Czech Republic) IC/CT4249/106

The subject-matter of this paper is the numerical simulation of the multidimensional inviscid compressible transonic gas flow. An adaptive mesh is constructed in the framework of the ADER higher order cell-centred finite volume scheme. An anisotropic mesh adaptation strategy is followed by a recovery of the approximate solution on the new mesh. The main feature of the proposed method is to keep the mass conservation of the numerical solution at each adaptation step. This allows the solution of non-stationary problems. The geometric conservation law is employed. The numerical solution for the case of a non-stationary discontinuity wave is presented. The algorithm consists of three basic sections at each time step: the time evolution of the numerical solution, the mesh adaptation and the recomputing of the numerical solution from the mesh before the adaptation to the mesh after the adaptation. In one time step the finite volume scheme is evaluated twice. Firstly for the prediction how to adapt the mesh, further for the update of the numerical solution itself. The two-dimensional numerical example employing the described higher-order method with proposed mesh adaptation is presented. The results from [1,2] are further extended.

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Non-reflecting boundary conditions for compressible Euler and Navier–Stokes equations in the finite-volume method. **Martin Kyncl** (Aeronautical Research and Test Institute, Czech Republic), Jaroslav Pelant (Aeronautical Research and Test Institute, Czech Republic), Jiří Felcman (Univerzita Karlova, Czech Republic) IC/CT4296/106

The paper is concerned with the numerical implementation of the inlet and outlet boundary conditions in the finite volume method for the solution of the 3D Euler and Navier-Stokes equations. The explicit time marching procedure is described. The classical Riemann problem is modified for physically relevant boundary conditions with the aim to keep conservation laws. This technique was used in [1]. The left hand right initial condition in the Riemann problem is replaced by the suitable one-sided boundary condition. This results in the acceleration of the numerical method itself. On the inlet the pressure and the density and the angle of attack or velocity vector and the entropy are prescribed. On the outlet the pressure or normal component of the velocity or temperature or mass flow are investigated in such a way to obtain the unique solution of the modified Riemann problem. Various combinations of inlet and outlet boundary conditions are investigated. This results in the sufficiently precise approximation of real flow boundary conditions. Numerical examples illustrating the usefulness of the proposed approach for cascade flow will be presented. Another numerical example was shown in [2]. This work was supported by the Grant MSM 0001066902 of the Ministry of Education of the Czech Republic. The authors acknowledge this support.

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Recent work on particle simulations. **Robert Krasny** (University of Michigan, Ann Arbor, USA) IC/CT3217/010

This talk will give an overview of recent work on particle simulations by the speaker and his collaborators. The approach taken here uses adaptive particle insertion, kernel smoothing, and a hierarchical treecode for regularized particle interactions. Applications in fluid, plasma, and molecular dynamics will be discussed. Work done in collaboration with Lyudmyla Barannyk, Hualong Feng, and Peijun Li (Michigan), Andrew Christlieb (Michigan State), Ben Sonday (Princeton), Leon Kaganovskiy (New College of Florida), and Hans Johnston (Amherst). Supported by the U.S. AFOSR and NSF.

Clustering of point vortices in a periodic box. **Makoto Umeki** (University of Tokyo, Japan) IC/CT4221/103

Motions of point vortices with periodic boundary conditions are studied by using Weierstrass zeta functions. We observe remarkable scattering and recoupling of vortex pairs when the vortex density is large. Clustering of point vortices with various initial conditions is quantitated with the L function which is used in point process theory in spatial ecology. Clustering in the initial conditions like an infinite row or checkered patterns is shown to persist during the numerical simulation.

Incompressible Navier–Stokes equation solvers based on lattice-Boltzmann relaxation systems. **Mapundi Banda** (University of KwaZulu-Natal, South Africa) IC/CT680/106

In this talk some recent numerical results based on discrete-velocity relaxation systems will be presented. Discrete-velocity equations are derived from continuous Boltzmann-type equations with appropriate approximations suitable for incompressible flows. A relaxation system is derived by taking moments of the discrete-velocity equations. Higher-order numerical discretizations of the relaxation system give higher-order discretizations of fluid flow equations. This approach is also extended to turbulent flows using Large-Eddy Simulation as well as thermal flows. The schemes are tested by solving a collection of examples. In particular the developed methods demonstrate potential as tools for Large Eddy Simulation and flow with Radiative Heat Transfer.

Higher-order semi-implicit discontinuous Galerkin finite-element method for the solution of the compressible Navier–Stokes equations. **Vít Dolejší** (Univerzita Karlova, Czech Republic) IC/CT3457/104

We deal with a numerical solution of the compressible Navier–Stokes equations with the aid of higher order schemes. We employ a combination of the discontinuous Galerkin finite element method for the space semi-discretization and a backward difference formula for the time discretization. Moreover, using a linearization of inviscid as well as viscous fluxes and applying a suitable explicit extrapolation for nonlinear terms we have to solve only a linear algebraic problem at each time step. Then we obtain an efficient numerical scheme which is almost unconditionaly stable and has a higher degree of approximation with respect to the space and time coordinates. We discuss some aspects of a stabilization, boundary conditions and an implementation. Several numerical examples are presented.

IC/CTS4935/10: Special/porous.

Organiser: Alaeddin Malek (Tarbiat Modares University, Iran)

Modeling of non-equilibrium phenomena in multiphase flow in porous media using stochastic particles. **Manav Tyagi** (ETH Zürich, Switzerland), Patrick Jenny (ETH Zürich, Switzerland), Hamdi Tchelepi (Stanford University, USA) IC/CT2651/100

Recently, we developed a stochastic particle method (SPM) for modeling multiphase flow in porous media (Tyagi et al., GAMM 2006, Berlin and Tyagi et al., CMWR-XVI 2006, Copenhagen). A Lagrangian viewpoint is adopted, in which a particle belongs to a specific phase. Saturation of a phase is the ensemble or spatial (local) average of the particles belonging to that phase. We showed how one recovers the macroscopic Darcy scale transport equations by moving the particles with the appropriate rules. Such a frame-work allows an alternative (and in some cases more natural) modeling approach of multiphase flow in porous media and provides a consistent link between small and large scales. The method is particularly suited for modeling reactive transport involving non-equilibrium phenomena that are difficult to describe in a deterministic Eulerian framework.
In this work, we show how the SPM can be used to model non-equilibrium effects due saturation fluctuations at the pore scales. This experienced fine scale saturation is not resolved and is a stochastic particle property. For illustration purpose we consider a simple model in which the experienced saturation relaxes to the ensemble saturation according to a linear relaxation equation. In the limit of zero relaxation time, the experienced saturation becomes equal to ensemble saturation. We also derive a transport equation for the probability density function (PDF) of experienced saturation and obtain Eulerian equations for the mean experienced and ensemble saturations. Opposed to the SPM, the Eulerian system of equations is unclosed, and one needs to know either the full joint PDF or has to do additional modeling. A similar approach could be applied for modeling nonlinear chemical reactions by assigning a composition vector to each particle.

Numerical solutions to the dual-phase-lag problem heated by short-pulsed lasers in nano-scale metals. **Alaeddin Malek** (Tarbiat Modares University, Iran) IC/CT756/107

The modified Fourier's law incorporating with the conservation of energy leads to hyperbolic heat conduction equation. Although the HHCE can explain many metal termal behaviors, it also introduces some physically impossible solutions. Instead the dual-phase lag model is more general and allows either the temperature gradient to precede the heat flux or the heat flux to precede the temperature gradient. Mathematically, the DPL model contains a third-order mixed derivative with respect to time, in which makes it different from the traditional heat transfer problem. Both one layer and multilayered structure within the framework of DPL heat conduction model is studied numerically by finite difference, spectral method and latice Boltzman method. Numerical results are presented.

Rayleigh–Bénard convection in a dielectric liquid: time-periodic body force. **Annamma Abraham** (R.V. College of Engineering, Bangalore, India) IC/CT766/106

Exploration of effective mechanisms of controlling convection in dielectric fluids is incessantly going on and has multifarious applications. An important class of natural convection problems is concerned with the difficulty in avoiding convection in the earth's gravitational field even when the basic temperature gradient is uniform and interfacial instabilities can be ignored. In the case of natural or simulated microgravity studies, time-dependent acceleration of sufficient amplitude due

to maneuvers and inherent mechanical vibrations lead to convection. This is referred to as the g-jitter effect. Time-periodic Body Force (TBF) is an externally modulated control of internal convection and may be realized by vertically oscillating a fluid layer in a constant gravitational field. Problems such as these have relevance in crystal growth in extra-terrestrial environment and attempted laboratory simulations of the same. Benjamin and Ursell (1954) examined the effect of TBF on the existence of standing waves on the free surface of a liquid in a vessel. Gresho and Sani (1970) studied the effects of TBF on the stability of a heated fluid layer. The stability of viscoelastic fluids in a modulated gravitational field was investigated by Yang (1997). Recently Siddheshwar and Pranesh (1999, 2000) examined the effect of g-jitter for weak electrically conducting and electrically conducting micropolar fluids.We investigate the effect of small amplitude TBF on the onset of convection in a horizontal layer of dielectric fluid using the Venezian method [1969]. A linear stability analysis is performed. The results obtained are based on the assumption that the amplitude of TBF is small. When $\omega < 1$ (i.e., the period of TBF is large) the TBF affects the entire volume of fluid and hence the disturbances grow large. On the other hand, the effect of TBF disappears for large frequencies. This is due to the fact that the buoyancy force takes a mean value leading to the equilibrium state of the non-TBF case. In the TBF problem R_{2c} is a crucial quantity which determines whether TBF leads to sub-critical instability or not. The results of the study indicate that TBF or g-jitter leads to delayed convection Also for large frequencies the effect of TBF disappears.

Stability of flow past cylinder cascade. **Venkata Boppana** (University of Manchester, UK), Jitesh Gajjar (University of Manchester, UK) IC/CT1748/106

The primary motivation for the current work is to develop suitable techniques for studying the global instability of separation bubbles such as those occurring in the flow past a row of circular cylinders placed in a uniform stream or in the supersonic flow past a compression ramp. In many previous studies of the instability of separation bubbles, the basic flow is taken to be locally parallel and this is used as input into the stability analysis. Mathematically this is only appropriate when the disturbance wavelength is small compared to the distance over which the flow develops and this is not always the case. Nevertheless, in many studies conclusions stemming from such local analyses are extrapolated to generate conclusions about the global instability of the flow. This of course raises questions about the credibility of such results.

In the current work we have extended the methods used to compute the steady flow past a cascade of circular cylinders to study the instability of these flows by using a new numerical technique, which is a high-order finite difference in one direction and Chebychev collocation in the other direction. Before implementing this numerical method, a number of test cases have been used for validation. One such test case is the flow in a lid-driven cavity where the global instability frequencies are found to correlate closely with temporal simulations of the linearised unsteady equations using forced disturbances. This led us to extend our techniques to study the instability of the flow in a cylinder cascade.

Numerical experiments were carried out on various grid sizes to check the convergence of critical parameters causing instability. The study also involved the computations with different locations of downstream boundary and varying blockage in order to understand their effect on critical Reynolds number (Re_c) and the associated Strouhal number (St_c). It is found that the primary instability in the wake for flow past cylinder is found to be due to a Hopf bifurcation and the values of Re_c and St_c are found to be 48.8 and 0.11806. It is also observed from the results that the blockage is significant in determining when the flow loses stability.

IC/CTS4823/10: Fluid dynamics related to biology and geosciences.

Organiser: Ali Nadim (Claremont Graduate University, USA)

An embedding method for simulation of immobilized enzyme kinetics and transport within sessile hydrogel drops. **Ali Nadim** (Claremont Graduate University, USA), Chao-Jen Wong (Claremont Graduate University, USA) IC/CT3069/107

A newly-developed embedding method for simulating enzyme kinetics and transport occurring within axisymmetric 3D domains is presented. The physical problem is pertinent to gel-pad microarrays for assessment of enzymatic activity. An enzyme is immobilized uniformly within a hydrogel which is spotted onto a solid surface in the form of a sessile drop, taking on a spherical cap shape. An aqueous solution containing substrate flows slowly past the porous drop. The substrate diffuses into the drop and is converted to product with the help of the enzyme. The product accumulates in and diffuses out of the drop and is taken away by the flow. Spatiotemporal distribution of the product, monitored via fluorescence, can be used to quantify the enzyme kinetics. This process is described by a system of nonlinear reaction-diffusion partial differential equations, modeling the diffusive transport and enzymatic reaction. The computational domain contains both the hydrogel drop and the bulk fluid phases. The embedding method is a computational technique that enables the use of finite differences on a regular Cartesian grid for simulation of multiphase problems with complex interfaces/boundaries. It uses a volume-fraction-based approach, similar to the volume-of-fluid (VOF) method, to implement the boundary conditions that must be applied at the interface between the phases. The main advantage of the embedding method is its simplicity, which results in code generation that can be highly optimized. In the present work, we apply the embedding method to the aforementioned two-phase reaction-diffusion problem and validate the results by comparing to a number of exact solutions available in simpler geometries and to results obtained using a finite-volume method on an unstructured body-fitted mesh.

Chocked flows in open capillary channels. **Jörg Klatte** (Universität Bremen, Germany) IC/CT1854/101

Capillary systems provide a passive means to control fluids and are widely used for space craft fuel management. In the present study the forced liquid flow through an open capillary channel under low gravity conditions is investigated.

Due to convective and viscous momentum transport the pressure along the flow path decreases and causes the free surface to bend inwards. Furthermore the free surface has a high tendency to oscillate due to minor flow perturbations. The maximum flow rate is achieved when the free surface collapses and gas ingestion occurs. This critical flow rate depends on channel geometry and liquid properties.

The talk concludes unsteady analytical modeling and numerical computations to calculate pressure, free surface curvature or velocity parameters. The results predict the critical flow rate for different geometries and can be used to avoid greater design margins of capillary systems.

Ultrasound propagation through blood containing microbubbles. **Sarah McBurnie** (University of Oxford, UK), Jon Chapman (University of Oxford, UK) IC/CT4413/103

In some types of diagnostic imaging, microbubbles (or ultrasound contrast agents) are injected into the blood to improve the backscatter from blood tissue in a way that enhances and improves the ultrasonic scan image generated. If an improved model for the acoustic scattering can be derived, then the image generated could be further improved.

Blood containing microbubbles is modelled as a bubbly fluid through which an acoustic wave is travelling. Nonlinear effects due to resonant bubble oscillations and bubble–bubble interactions are examined using asymptotic and homogenisation techniques.

Adaptive simulation of fluid–propagule interaction: application to the settlement of seaweed zygotes. **Sébastien Delaux** (NIWA/University of Canterbury, New Zealand), Stephane Popinet (Nat. Inst. of Water and Atmospheric Research, New Zealand), Craig Stevens (Nat. Inst. of Water and Atmospheric Research, New Zealand) IC/CT4500/105

Many phenomena in nature involve a wide range of scales, some of the small scales being sometimes located in regions of restricted size. The numerical study of a multi-scale flow requires the use of a mesh refined enough to solve the smallest scales. Also, problems involving static or moving solid boundaries necessitate an accurate representation of the solid objects involved. This often means that a fine mesh is needed near the solid boundaries. In these cases, the use of adaptive mesh refinement techniques can be very useful.

Both a wide range of scales and solid boundaries are involved in the modelling of the settlement process of seaweed zygotes. New Zealand intertidal seaweeds reproduce by releasing eggs and sperm to the nearshore environment. Once fertilized, seaweed propagules have to reach a suitable substrate and attach. Very little is known about the processes governing attachment and detachment of these propagules, particularly in turbulent wave-driven coastal waters. A critical part of the attachment/detachment process occurs in the turbulent viscous boundary layer near the substrate.

In order to study numerically this problem, a solid/fluid interaction model is being implemented in the Gerris Flow Solver (http://gfs.sf.net). Gerris solves the 2D/3D incompressible Navier-Stokes equations using a finite volume formulation. Gerris is based on a quadtree/octree mesh, adaptive in space and time.

The spatial and temporal adaptivity of the code will allow us to resolve the small eddies and to follow them without spending too much computer power on the rest of the domain. As we are ultimately aiming at doing some 3D simulations, the adaptivity is crucial.

I will mainly present the numerical work done to develop the solid/fluid interaction model in the Gerris Flow Solver. The methods used to implement and validate this model will be exposed in detail. Applications related to the attachment process of seaweed propagules will be presented.

Evolution of solitary marginal disturbances in baroclinic frontal geostrophic dynamics with dissipation and time-varying background flow. **Edwin Swaters** (University of Alberta, Canada) IC/CT4202/102

The finite amplitude evolution of solitary disturbances in baroclinic frontal geostrophic dynamics in the presence of time-varying background flow and dissipation is shown to be governed by a 2-equation extension of the *unstable* nonlinear Schrödinger (UNS) equation with variable coefficients and forcing. The soliton solution of the unperturbed UNS equation corresponds to a saturated isolated coherent anomaly in the baroclinic instability of surface intensified oceanographic fronts and currents. The adiabatic evolution of the propagating soliton and the uniformly valid first-order perturbation fields are determined using a direct perturbation approach together with phase-averaged conservation relations when both dissipation and time-variability are present. It is shown that the soliton amplitude parameter decays exponentially due to the presence of the dissipation but is unaffected by the time variability in the background flow. On the other hand, the soliton translation velocity is unaffected by the dissipation and evolves only in response to the time variability in the background flow. The adiabatic solution for the induced mean flow exhibits a dissipation-generated "shelf region" in the far field behind the soliton, which is removed by solving the initial-value problem.

Multicloud models for tropical convections and convectively-coupled waves. **Boualem Khouider** (University of Victoria, Canada) IC/CT4059/107

Tropical convection and convectively coupled waves have a big impact on our day to day weather and climate. The so called Madden–Julian or intra-seasonal oscillation is believed to effect many important climate and weather patterns such as El-Niño Southern Oscillation, the Asian and Australian monsoons, and the tropical–extratropical tele-connection patterns. Despite the progress in super-computing, the general circulation models (GCM) used for long-term weather and climate predictions at best perform poorly in representing these important tropical waves. This poor performance is partly due to the multiscale nature of these waves and the strong interactions across time and length scales between the individual clouds and the large-scale circulation.

Idealized models with a crude vertical resolution reduced to one to two vertical baroclinic modes are commonly used for both theoretical and numerical studies. Recent analysis of observational data reveals that three cloud types are involved in tropical convection; shallow-non precipitating cumulus clouds, congestus clouds, and deep convective hot-towers expanding in the upper troposphere into stratiform anvils. We propose a new family of multicloud convective parametrization using three cloud-types. Congestus clouds heat the lower half of the troposphere and cool the upper half, while deep convective clouds heat the entire troposphere. Stratiform clouds on the other hand heat the upper troposphere and cool the lower troposphere through evaporation of rain falling into dry air. The resulting phenomenological model is then analyzed both by linear stability theory and non-linear simulations. It is found that the multicloud models capture many key observed features of convectively coupled waves in the tropics.

This is joint work with Andrew J. Majda (NYU).

IC/CTS4934/10: Numerical methods.

Comparison of different techniques for the study of nonlinear laminar flow between parallel perforated disks. **P A Dinesh** (MSRIT, Bangalore, India), Karthik Adimurthi (M.S.Ramaiah Institute of Technology, India) IC/CT25/106

The equations describing similarity solutions for the flow between infinite parallel perforated disks with equal rates of suction or injection at the interface are analyzed. The nonlinear ODE is found to admit a solution for all Reynolds numner (R) using Leray Schauder degree theory. Uniqueness of solution for small Reynolds number is proved analytically. The nonlinear ODE is then solved computationally using regular perturbation technique, numerical finite difference scheme and Padé approximation. From numerical simulations, it is found that regular perturbation method and numerical finite difference

scheme fail for larger values of R, whereas Padé approximation gives converging solution for all values of R and this solution shows the disappearence of boundary layer as $R \to \infty$, and as a consequence shock is developed. For practical applications, the coefficient of skin friction and pressure distribution are also calculated.

Influence of low Mach numbers on the numerical dissipation of Godunov-type schemes. **Felix Rieper** (TU Cottbus, Germany) IC/CT2274/106

We present a new method for analysing the accuracy problem of first-order upwind schemes for the Euler equations in the low Mach number regime. The analysis makes use of the modified equation approach and, with the new concept of *numerical Reynolds numbers*, allows the classification of Riemann solvers and flux vector splittings into two categories: adequately and excessively dissipative.

Roe's approximate Riemann solver is shown to be of the first category, keeping a balance between physical convection and artificial dissipation for all characteristic waves independent of the Mach number. Further members of this class are HLLC and the original Godunov scheme. Correct flow simulations with an $\mathcal{O}(\mathrm{M}^2)$-pressure field for Mach numbers as low as $\mathrm{M} = 10^{-6}$ confirm the analysis.

HLL is shown to become more and more dissipative for low Mach numbers, leading to highly viscous flow that resembles *Stokes* or *creeping flow* with an $\mathcal{O}(\mathrm{M})$-pressure field. Numerical results verify this analogy. This class of upwind schemes with excessive numerical dissipation is shown to comprise the flux vector splittings of van Leer and Steger–Warming.

A novel pressure decomposition into physically and numerically induced pressure variations explains the different order of magnitudes of pressure fields, observed for the two classes of upwind schemes in this flow regime.

Adaptive least-squares finite-element approximations to transonic-flow problems. **Tsu-Fen Chen** (National Chung Cheng University, Taiwan), Shin-Perng Chang (Toko University, Taiwan) IC/CT4726/010

This work concerns solutions of compressible potential flow problems based on weighted least-squares finite element approximations. The model problem considered is that of the potential flow past a circular cylinder. To capture the transonic flow region, an adaptive algorithm based on mesh redistribution with local mesh refinement and smoothing is developed for suitably weighted least-squares approximations. Numerical results for the model problem are given for both subsonic and transonic cases.

Mixed finite approximation of a coupled reservoir–well-bore problem with heat transfer. **Layal Lizaik** (Université de Pau et des Pays de l'Adour, France), Mohamed Amara (Université de Pau et des Pays de l'Adour, France), Daniela Capatina-Papaghiuc (Université de Pau et des Pays de l'Adour, France) IC/CT2005/025

We are interested in the thermomechanical coupling of a petroleum reservoir with a vertical wellbore, both written in 2D axisymmetric form, in order to interpret recorded temperatures in the wellbore as well as a flowrate history and thus to better characterize the reservoir. The reservoir is assumed to be a monophasic porous medium, described by the Darcy-Forchheimer equation together with a non standard energy balance which includes viscous dissipation and compressibility effects. Concerning the wellbore, which is a compressible fluid medium based on the Navier-Stokes equations, a 1.5D model is derived as a conforming approximation of the 2D axisymmetric one. In order to couple the two models, adequate transmission conditions at the perforations are imposed and next dualized by means of Lagrange multipliers. We obtain, at each time step, a mixed formulation binding together the two formulations of the separated models. Mathematically, its operator is non standard and the uniqueness of the solution is established by means of a generalization of the Babuška-Brezzi theorem. A global solving of the coupled problem is then envisaged. Concerning the spatial discretization, we approximate the heat and mass fluxes by the lowest-order Raviart-Thomas mixed elements, the pressure and the temperature by piecewise constant elements, the fluid's velocity by Q_1 continuous elements while the Lagrange multipliers on the interface are taken piecewise constant. The convective terms are treated by appropriated upwind schemes. A technical analysis of the discrete mixed formulation is carried on and the well-posedness of the problem is proved. This result is used to show the existence of a solution for the continuous coupled problem by a Galerkin method. Numerical tests including real cases as well as a comparison with the results obtained separately by the two models will be presented. This work is supported by TOTAL.

Preconditioners for hydropower plant reservoir flow simulations. **Norberto Mangiavacchi** (Universidade do Estado do Rio de Janeiro, Brazil), Luiz Carvalho (Universidade do Estado do Rio de Janeiro, Brazil), Cassio Soares (Furnas Centrais Elétricas S.A., Brazil), Virginia Costa (Universidade do Estado do Rio de Janeiro, Brazil), Wagner Fortes (Universidade do Estado do Rio de Janeiro, Brazil) IC/CT2534/103

The incompressible Navier–Stokes equations are solved employing Finite Element approximations for the simulation of hydroelectric power generation reservoir flows. We present different approaches for the solution of the coupled velocity-pressure algebraic equations. In the first approach, an approximate block Cholesky factorization is employed, which reduces the problem to the solution of two uncoupled SPD systems, which are solved using the PCG method, with incomplete Cholesky preconditioners. In the second one, the system is solved employing the GMRES method. For this method, several preconditioning strategies are compared. One of the choices of preconditioning is based on the block Cholesky factorization of the uncoupled problem. The preconditioners are implemented using Trilinos and the main code is written in C++, using an Object Oriented approach. For the computational kernels, combinations of optimized sparse and dense BLAS are implemented. Results are discussed.

This work was developed at GESAR Labs (UERJ, Rio de Janeiro, Brazil), with financial support from FURNAS CENTRAIS ELÉTRICAS S.A., CAPES and CNPq.

Variational method in the unified coordinate system. **Guiping Zhao** (IAPCM, Beijing, PR China) IC/CT2089/106

How to establish the equation of the arbitrary parameter h, which is introduced into the fluid dynamic equations in the unified coordinate system, is very important in simulating the multi-material flow. On the interface between the different materials which we are interested in, the h value should be 1 so that we can obtain Lagrange solution. In the unified coordinate system, the h equation is hyperbolic, and h value canŠt be fixed on all boundaries. In this paper, variational method is used to form the elliptic h equation, and the mesh spacing, smoothness, orthogonality and regularity of grid generated are also considered. Some typical examples demonstrate that variation method used in the unified coordinate system is possible, and

the distribution of h can be adjusted by given different boundary conditions, so as to get adaptive meshes for idiographic physical problems.

Key words: Unified coordinate system, h-equation, Variation method, Interface

IC/CTS4831/10: Cavitating flow, porous media, boundary layers and cavity flow.

Re-entrant corner flows of Phan-Thien-Tanner fluids. **Jonathan Evans** (University of Bath, UK) IC/CT4786/103

Steady planar flow of the Phan-Thien-Tanner (PTT) fluid is described for re-entrant corners with angles π/α where $1/2 \leq \alpha < 1$. Local to the corner we consider a class of similarity solutions associated with the inviscid flow equations which arise from the dominance of the upper convective stress derivative in the constitutive equations. These solutions hold in an outer (core flow) region and give stress singularities of $O(r^{-2(1-\alpha)})$ (with r the radial distance from the corner) and a stream function behaviour of $O(r^{n\alpha})$. Here n is a parameter defining distinct solutions within this similarity class. We match such solutions to inner regions at the walls (i.e. wall boundary layers), in which viscometric behaviour is retrieved and which determines $n = 1 + \alpha$. The formulation is carried out using both the Cartesian and natural stress basis and it is implicitly assumed that there are no regions of recirculation at the upstream wall i.e. we consider flow in the absence of a lip vortex. In this situation, a two parameter family of solutions is described for the local asymptotic behaviour of the flow and stress fields. Essential features of the analysis are the matching of the core region to the wall boundary layers, the solution (numerical and asymptotic) of the upstream and downstream boundary layers, together with the explicit determination of the essential singularity possessed by the boundary layer equations at the downstream wall.

Such re-entrant corners arise naturally in planar or axisymmetric contraction flows and are standard problems for the testing of numerical methods. However, the stress singularities that arise pose numerical difficulties, particularly near to and downstream of the corner for a wide class of elastic fluids (the PTT fluid being one such type).

Numerical simulation of non-classical waves for immiscible three-phase flow in heterogeneous porous media. **Eduardo Abreu** (Universidade do Estado do Rio de Janeiro, Brazil) IC/CT616/100

We describe the development of a numerical simulation tool for three-phase immiscible incompressible flow. The porous medium may be heterogeneous, including variable permeability and porosity fields, and general relations for the relative permeability functions may also be used. The latter may lead to the loss of strict hyperbolicity and, thus, to the existence of an elliptic region or an umbilic point for the system of nonlinear hyperbolic conservation laws describing the convective transport of the fluid phases. This numerical procedure has been used to investigate the existence and stability of nonclassical waves (also called transitional or undercompressive waves) in heterogeneous two-dimensional flows, thereby extending previous results for one-dimensional problems. Preliminary results concerning the investigation of gravity effects on three-phase flows will be also presented. Work done in collaboration with: Fred Furtado (UWYO/USA), Dan Marchesin (IMPA/BRAZIL) and Felipe Pereira (UERJ/BRAZIL).

Numerical study of transient natural convection in a cavity with multiple adiabatic blocks. **Durga Charan Dalal** (IIT Guwahati, India), Swapan Pandit (IIT Guwahati, India) IC/CT2947/107

This study deals with the solution of a problem of unsteady natural convection in a thermally driven square enclosure with four adiabatic square blocks placed inside. In this problem, vertical walls are assumed to be adiabatic and horizontal walls are differentially heated where the lower wall is hot and the upper one is cold. A fourth-order accurate compact scheme which is spatially fourth order and temporally second order accurate has been employed on a nonuniform grid to numerically solve the governing equations. A detailed study of transient flow structure and heat transfer in the presence of four adiabatic blocks for different Rayleigh numbers (mainly, ranging from 10^3 to 10^6) has been made.

In order to validate the code, our results have been compared with those of Davis [*Int. J. Numer. Methods Fluids* **3**, 249, 1983] (known as benchmark results) and found an excellent agreement. The numerical results corresponding to the steady state fluid flow and temperature fields at $Ra = 10^3$ show the four symmetrical zones around four blocks. For $Ra = 10^4$ and 10^5, the flow and temperature fields reach their steady-state after some decaying oscillatory transient. Flow and temperature fields for $Ra = 10^6$ or higher, are quite different. [Our study has not yet been fully completed.]

Super-critical withdrawal from a two-layer fluid in a porous medium. **Graeme Hocking** (Murdoch University, Australia) IC/CT4178/101

During withdrawal of oil below gas, or fresh water from above salty in a porous medium, there is a critical flow rate above which both layers begin to flow into the outlet. Numerical calculations of the interface shape (and critical values) indicate that the critical flow value obtained is either much lower than earlier hodograph techniques suggest or is accompanied by a sudden jump in the shape of the dividing boundary.

On analogy of effect of random errors to several stabilizing terms in flow simulations. **Itaru Hataue** (Kanazawa University, Japan) IC/CT1182/106

TThe complicated phenomenon such as flow motions can be simulated easily as if they were open before our eyes actually. However, nobody can confirm whether computed results reliable or not. This is responsible for the strong nonlinearity induced by insertion of random errors. In this paper, we studied the structure of numerical solutions of flow simulations in order to clarify effects of such insertion of random errors. Concretely, we investigate the characteristics of asymptotic numerical solutions which are given by solving incompressible Navier Stokes equations directly. The incompressible Navier-Stokes equations and the continuity equation are solved numerically by using the MAC(Maker-And-Cell) method and implicit temporal scheme. The model adopted in the present study is a flow around a two-dimensional circular cylinder and the Reynolds number is 1500. We must introduce the higher order artificial viscosity terms in order to perform the calculations stably and we get multiple stable asymptotic solutions by selecting the amplitude of the artificial viscosity tems. Though the numerical fourth order artificial viscosity has the stabilizing effect like the physical second order one, the bifurcation processes are different. On the other hand, we studied influences of structure of numerical solutions which are given by solving the Navier-Stokes equations numerically on amplitude of added randomness. Random noises are given by using pseudo-random number. As the result, we found that characteristics of asymptotic solutions change under the condition of insertion of random noises. This phenomenon may relate to the stochastic resonance or the entrainment phenomena. Further-

more, we discussed the analogy of effect of Random errors to several stabilizing terms in flow simulations in the present study. Concretely, we concentrate the dependence of bifurcation processes on the amplitude of fourth order viscosity terms and that of added random errors. It was shown that relatively large random errors stabilize the system and havw the similar effect of stabilizing viscosity terms. Furthermore, dependence of stability of attractors on several types of insertion of random errors is discussed.

Oblique water-wave scattering by a small undulation on a porous sea-bed. **Subash Martha** (IIT Guwahati, India), Swaroop Bora (IIT Guwahati, India) IC/CT429/101

Almost all the existing investigations on the wave reflection and/or transmission problems of porous structures are investigated by assuming horizontal sea-bed. However, in practical coastal engineering, an undulating sea-bed is more likely to be encountered for the interaction with wave motion. The problem of scattering of two dimensional surface water waves by small undulation on a sea-bed of finite depth is considered here assuming the sea-bed to be composed of porous material of specific type. The governing boundary value problem (BVP) is reduced to a simpler BVP for the first order correction of the potential using perturbation analysis which involves a small parameter ϵ present in the representation of the small undulations on the porous sea-bed. Fourier transform method is utilized to obtain the complete solution of the mixed boundary value problem, under the assumption that the undulation of the sea-bed is small enough so that a regular perturbation expansion in terms of a small undulation parameter is applicable. The reflection and transmission coefficients are determined and applied to the case of a patch of sinusoidal undulations on the bed. When the ripple wave number (l) is equal to twice the $x-$component (μ) of the surface wave number, the first order reflection coefficient is found to increase when the bed has more porous effect. When there is no porous effect on the sea-bed it is found that the present results resemble the ones obtained earlier by Davies and Heathershaw (1984) for surface wave propagation over sinusoidally topography. The results are presented in graphical forms. The case of oblique incidence is handled completely.

IC/CTS4932/10: Interior flow, flow about cones.

Application to Noshiro's ventilation system. **Masao Igarashi** (Nihon University, Japan), Yukio Yanagisawa (Nihon University, Japan), Cheng Yen Tsai (Nihon University, Taiwan), Makoto Murofushi (Osaka University, Japan) IC/CT3968/010

Nearly one hundred years ago, in 1910, K. Noshiro invented a buoyancy-driven natural ventilation system which controlled the temperature of a malted rice room called *Koj*' room to be almost constant and contribute to produce high-quality rice-wine called Sake.

He installed two different-length chimneys at the top of the room to control the temperature. The shorter chimney supplies cooler air into the room, on the other hand the longer chimney releases warmer air from the room. The system controlled the temperature of the room adequately, so that the high quality of Sake was produced.

We propose a new buoyancy-driven natural ventilation system which consists of just one chimney. The top of the chimney is not flat, but slope. The slope creates a circulation of heat between the room and outside, that is, the taller side of the chimney releases the warmer air from the room and the shorter side supplies the cooler air into the room. The difference between the taller side of the temperature and the shorter side of the temperature is increasing with decreasing the width of the chimney. However for a very small width, the temperature at the both sides is closed together.

We propose a chimney whose top is angled and show that the chimney makes a natural ventilation. We also consider the effective angle of the chimney to arise the natural ventilation.

Axisymmetric and non-axisymmetric flow modes between rotating coaxial cones. **Christopher Hills** (Dublin Institute of Technology, Ireland) IC/CT2160/105

We consider the slow flow of a fluid contained in the conical cavity formed between two coaxial cones with coincident apices. The fluid is set in motion by the rotation of the conical boundaries or a bounding spherical lid. The Stokes flow is laminar but at higher orders a meridional circulation is induced due to the sloping boundaries. This meridional circulation can exhibit recirculation regions or eddies for determined constraints upon the geometrical and dynamical parameters. The three-dimensional slow flow can thus be exploited in the manufacture of pumps, particularly in the medical sciences, and has implications for the mixing of viscous fluids in this geometry.

Truncated two-cone geometries have been previously studied experimentally but there are relatively few theoretical treatments of the full two conical geometry. Eddies can occur in the cavity of a single fluid filled cone for apex angles less than a critical value, but it is found that the addition of a second cone has a dramatic effect upon this critical angle.

We investigate the presence of eddies due to the dominance of flow components associated with the geometry over forced flow effects. A variety of driving mechanisms is studied where the conical boundaries and spherical lid are allowed to rotate independently with particular attention to the destruction of eddies by shearing and overall rotation. Eddies can also arise due to symmetries of the driving mechanism. We extend our previous analyses by also considering non-axisymmetric flow modes. It is shown that the dominant flow mode is associated with non-zero azimuthal wave numbers and that cascades of eddies can be guaranteed.

Work done in collaboration with O. Hall & A.D. Gilbert, University of Exeter, UK.

Effect of pressure work on free convection flow along a vertical circular cone with suction and variable surface temperature. **Md Abdul Alim** (Bangladesh University of Engineering & Technology) IC/CT781/010

Free convection laminar flow from a vertical circular cone maintained a variable surface temperature with suction and pressure work effects has been investigated. The governing boundary layer equations are transformed into a non-dimensional form and the resulting nonlinear system of partial differential equations are reduced to local non-similarity equations. The governing non-similarity equations are then solved numerically by Implicit finite difference method together with Keller box scheme. Numerical results are presented in terms of velocity and temperature profiles of the fluid as well as the local skin-friction coefficients and the local heat transfer rate for different values of Prandtl number $\Pr$, suction parameter ξ, temperature gradient parameter n and the pressure work parameter $\in$.

Optimal control of flows in moving domains. **Bartosz Protas** (McMaster University, Canada), Wenyuan Liao (McMaster University, Canada), Donn Glander (General Motors Research & Development Center, USA) IC/CT2599/105

This investigation concerns adjoint-based optimization of viscous incompressible flows (the Navier–Stokes problem) coupled with heat conduction involving change of phase (the Stefan problem) and occurring in domains with moving boundaries such as the free and solidification surfaces. This problem is motivated by optimization of advanced welding techniques used in automotive manufacturing, where the goal is to determine an optimal heat input, so as to obtain a desired shape of the weld pool surface upon solidification. This will guarantee good properties of the resulting joint. In order to use a gradient based optimization approach, it is necessary to characterize the sensitivity (i.e., the gradient) of the cost functional with respect to the control (the heat input). This can be done conveniently using suitably-defined adjoint equations. A difficulty in the present problem is that the shape of the domain is also a dependent variable, and both the cost functional and the state variables need to be differentiated with respect to evolution of the domain. This is accomplished using methods of *non-cylindrical* calculus which allows us to derive a perturbation system accounting for domain variability. An adjoint system is derived afterwards which, unlike the forward problem, is defined on a domain with a predetermined evolution in time and also involves ordinary differential equations defined on the domain boundary (*the adjoint transverse system*). In our presentation, after formulating the optimization problem, we will review basic elements of the non-cylindrical calculus and show how it can be used to derive the perturbation system. For the sake of clarity, these derivations will be analyzed using a simpler model problem involving a 1D heat equation in a variable domain. Finally, we will discuss certain computational aspects of numerical solution of such adjoint problems and will present numerical results concerning both the model and the original problem.

IC/CTS4975/10: Special fluids.

Organiser: Mehmet Pakdemirli (Department of mechanical Engineering, Celal Bayar, Turkey)

Solutions of a generalized hyperbolic non-Newtonian fluid flow for special geometries. **Mehmet Pakdemirli** (Department of mechanical Engineering, Celal Bayar, Turkey), Pinar Sari (Celal Bayar University, Turkey), Bekir Solmaz (Celal Bayar University, Turkey) IC/CT1102/103

A generalized hyperbolic non-Newtonian fluid model is considered. The model was successfully applied to some drilling fluids with better performance in relating shear stress and velocity gradient compared to power-law and Hershel-Bulkley model. Special flow geometries namely pipe flow, parallel plate flow and flow between rotating cylinders are treated. For the first two cases, analytical solutions in the form of integrals are presented. The velocity profiles and discharge are calculated by numerically evaluating the integrals. For the flow between rotating cylinders, the differential equation is solved by Runge-Kutta method combined with shooting.

Optimizing the source distribution in fluid mixing. **Jean-Luc Thiffeault** (Imperial College London, UK), Grigorios Pavliotis (Imperial College London, UK) IC/CT2184/107

Consider a passive scalar advected by a velocity field, and assume the concentration of the scalar is continually replenished by a spatial source. For example, we could have a source of heat with hot and cold spots, such that the mean temperature is constant. An obvious question is, which velocity fields are best at homogenizing the concentration field? This is a challenging question, and here we turn it around into a less obvious one: given a velocity field, which source distributions are best mixed by this field? This question is simpler to answer and yet is relevant to real mixing problems. We use a multiscale measure of steady-state mixing efficiency [1,2], similar to the mix-norm [3], and optimize it using a variational approach. We then solve the resulting Euler–Lagrange equation for a simple cellular flow. The optimal source distributions have many gross features that are as expected: they favor fast regions of the flow, and their contours are aligned such that the flow blows hot spots onto cold spots and vice versa. However, the detailed structure varies widely with diffusivity and other problem parameters. Though this is a toy problem, the procedure is easy enough to be adapted to more complex situations.

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Large-scale simulation of shock- and detonation-driven fluid-structure interaction phenomena. **Ralf Deiterding** (Oak Ridge National Laboratory, USA) IC/CT3232/105

The impact of shock or detonation waves on solid materials can induce large structural deformations, fracture and fragmentation. Coupled fluid-structure interaction simulations are very challenging, because numerical methods have to cope with complex topology evolutions. We present an approach to coupling that uses a level set function for implicit geometry representation and is particularly robust [1].

The compressible fluid flow is simulated with a high-resolution shock-capturing Cartesian finite volume upwind method in Eulerian coordinates that considers the solid as a moving embedded body based on the current level set information. The structural response is calculated with problem-specific finite element schemes in Lagrangian coordinates. A loosely coupling temporal splitting method is applied to update the boundary's positions and velocities between time steps. The Eulerian finite volume scheme is incorporated into a parallel structured dynamic mesh adaptation algorithm that allows very fine local resolutions to capture the near-body interaction and incoming waves in the fluid at minimal computational costs. As the solid deforms, the level set function storing the distance to the solid surface is updated on-the-fly by a highly efficient auxiliary algorithm that utilizes geometric characteristic reconstruction and scan conversion.

As large-scale, three-dimensional computational examples we consider the deformation of a metal container due to the combustion of a high-energetic solid explosive, the rupture of thin aluminum tubes induced by interior gaseous detonations, and the deformation of copper plates under water hammer. Briefly, the software design and the parallelization of all components for distributed memory computing platforms are sketched.

This work is sponsored by the Mathematical, Information, and Computational Sciences Division; Office of Advanced Scientific Computing Research; U.S. Department of Energy and was performed at the Oak Ridge National Laboratory, which is managed by UT-Battelle, LLC under Contract No. De-AC05-00OR22725.

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Direct numerical simulation of turbulent visco-elastic flows: dynamic Karhunen–Loeve analysis. **Antony Beris** (University of Delaware, USA), Gaurab Samanta (University of Delaware, USA) IC/CT4556/103

Polymer-induced turbulent drag reduction has been the subject of intense investigations ever since its accidental discovery by Tomms and Mysels during the Second World War, with important applications, most well known of which is the facilitation of the oil transfer though pipelines, such as in the Alaskan pipeline. Recent developments in numerical methods, and more specifically an exponential mapping for the viscoelastic conformation tensor that allows us to preserve its positive definiteness under all flow conditions exactly, allowed us to obtain accurate and stable simulations up to highly drag reduced (more than 60%) turbulent channel flows of dilute polymer solutions. The most recent data confirm earlier results in our group at lower drag reduction values whereby the primary mechanism for drag reduction is the decreased intensity of the wall eddies which is the result of a significant increase to extensional deformations contributed by the polymer additives, exactly as proposed earlier by Metzner and Lumley. Recent work has been able to more systematically investigate the changes to the flow structure effected due to the polymers, and in particular the coherent structures, using Karhunen-Loeve (K-L) Proper Orthogonal Decomposition (POD) analysis of the data. This demonstrated a dramatic enhancement of the importance of large scale motions with increased viscoelasticity and an equally dramatic decrease in the K-L dimension of the flow (an order of magnitude) as viscoelasticity increases versus similar Newtonian results. Moreover, the time-dependent dynamic analysis of the solution in terms of the K-L modes has confirmed the increased time scales encountered with viscoelasticity and has proven useful towards establishing a better understanding of the turbulent coherent structures and their interrelationships as they have been modified by viscoelasticity.

IC/CTS4830/10: Reactive flows and heat transfer.

Organiser: Ilya Simanovskii (Technion – Israel Institute of Technology)

Finite-element method simulation of rotating disk flow: effect of the transport of a chemical species. **José Pontes** (Universidade Federal do Rio de Janeiro, Brazil), Gustavo dos Anjos (Universidade do Estado do Rio de Janeiro, Brazil), Norberto Mangiavacchi (Universidade do Estado do Rio de Janeiro, Brazil) IC/CT3158/103

We consider the stability of rotating disk flow coupled, through the fluid viscosity, to the mass concentration field of a chemical species. This configuration refers to an electrochemical cell with an working electrode consisting of an iron rotating rod which is dissolved in the electrolyte, a 1 $\mathbf{M}$ $\mathbf{H_2SO_4}$ solution. Polarization curves obtained in such cells present a current instability at the beginning of the region where the current is controlled by the mass transport. The instability appears at a certain value of the applied potential and is suppressed beyond another value. Dissolution of the electrode gives rise to a thin concentration boundary layer, which, together with the potential applied to the electrode, results in an increase in the fluid viscosity and in a decrease in the diffusion coefficient, both affecting the current. This work deals with the question of whether the current instability may originate from an instability of the coupled fields, namely, if the coupling reduces the critical Reynolds number to values comparable to those attained in experimental setups. A phenomenological law is assumed, relating the fluid viscosity to the concentration of a relevant chemical species. Parameters appearing in this law are evaluated on basis of experimental electrochemical data.

The Finite Element Method (FEM) is employed to solve the coupled incompressible Navier-Stokes and chemical species transport equations, using a tetrahedral mesh. A semi-Lagrangian technique is used for the discretization of the material derivatives, and the spatio-temporal discretization is made through the implicit Taylor-Galerkin method,leading to an unconditionally stable scheme, suitable for large Reynolds and CFL numbers. Pressure and velocity are solved using a segregated LU factorization scheme. The resulting symmetric and positive-definite systems are solved by the Preconditioned Conjugate Gradient method. Good numerical stability properties were obtained with the proposed scheme and the results are in agreement with a linear stability analysis of the problem.

The authors acknowledge financial support from the brazilian agency CNPq.

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Numerical modeling of the hydrodynamic field coupled to the transport of chemical species through the finite-element method. **Gustavo dos Anjos** (Universidade do Estado do Rio de Janeiro, Brazil), Norberto Mangiavacchi (Universidade do Estado do Rio de Janeiro, Brazil), José Pontes (Universidade Federal do Rio de Janeiro, Brazil), Cassio Soares (Furnas Centrais Elétricas S.A., Brazil) IC/CT3133/101

The simulation of the complex fluid flow and transport in hydro-powerplant reservoirs requires the solution of the Navier-Stokes equations coupled, through the physical properties of the fluid, to the transport equation of chemical species and the energy equation. The purpose of this study is to develop a Finite Element Method for the simulation of the filling of hydropower plant reservoirs, in order to asses the environmental effects of the formation of the reservoirs and analyse possible strategies for remediation.

The domain is discretized employing a Delaunay Tetrahedralization algorithm, to guarantee good properties in the element mesh. Spatial discretization of the diffusion and pressure terms is made through the Galerkin method whereas the substantial derivatives are treated through a semi-Lagrangian technique that presents natural stability. The time discretization is done through a first-order backward Euler implicit scheme. The large systems of coupled linear equations are solved through the discrete projection method based on the LU decomposition, resulting in symmetric positive-definite system matrices. The method proved to be stable at all CFL and Reynolds conditions, not showing spurious oscillations or excessive numerical diffusion even under large Reynolds number conditions.

This work was developed at GESAR Labs, in the State University of Rio de Janeiro, Brazil, under the sponsorship of the brazilian power company FURNAS CENTRAIS ELÉTRICAS S.A., CAPES, and CNPq, from whom the authors acknowledge the support.

Nonlinear convective oscillations in multilayer systems. **Ilya Simanovskii** (Technion – Israel Institute of Technology) IC/CT548/107

During the last few decades, a new scientific direction of investigation, convection in multilayer systems, was developed. Among the modern techniques requiring an investigation of convection in systems with many interfaces are liquid encapsulation crystal growth technique used in space labs missions, droplet-droplet coalescence processes, where Marangoni convection in the interdroplet film can considerably affect the coalescence time during extraction, and others. A scientific interest in such systems is due to the fact that the interfacial convection in multilayer systems is characterized by a variety of physical mechanisms and types of instability (for a review, see A. Nepomnyashchy, I. Simanovskii, J.C. Legros "Interfacial convection in multilayer systems", Springer, New York, 2006).

In the present work some peculiarities of the instabilities in three-layer systems are investigated. It is shown that the oscillatory instability in multilayer systems is much more widespread that in a two-layer one. Direct and indirect interaction of different mechanisms of instability may lead to specific types of oscillations. The nonlinear simulations of the Marangoni convection in a symmetric three-layer system of fluids, 47v2 silicone oil – water – 47v2 silicone oil, have been performed. Different types of oscillatory motions, as well as transitions between nonlinear convective regimes, have been studied.

The joint action of buoyancy and thermocapillary effect on the convection in the three-layer system, air – ethylene glycol – fluorinert FC75, is investigated. The stability diagram on the plane the Grashof number – the Marangoni number, is constructed. It is shown that the region of the Grashof number values, where nonlinear oscillations take place, is bounded both from below, by the mechanical equilibrium, and from above, by the steady state.

Numercial simulations for a fluid in an elastic cylinder with two chambers. **Sunmi Lee** (Konkuk University, Republic of Korea), Eunok Jung (Konkuk University, Republic of Korea) IC/CT742/010

In this work, we construct a new model of valveless pumping for an elastic tube with two chambers. Mathematical modeling and numerical simulations of flows driven by periodic pumping are presented. A periodic compression of the assymmetric part of the soft tube generates a unidirectional flow. Both the amount and the direction of a net flow depend on the frequency and the compression of periodic pumping.

Optimal control on thermo-convective patterns. **Maria Cruz Maria Cruz** (Universidad de Castilla-La Mancha, Spain), Henar Herrero (Universidad de Castilla-La Mancha, Spain), Ana Mancho (Consejo Superior de Investigaciones Científicas, Spain) IC/CT3276/107

We study the optimal control and the linear stability of stationary thermally convected fluid flows induced by a horizontal temperature gradient and driven by the buoyant force. The control is effected through a heat flux on the top boundary. The control problem is formulated as a constrained minimization problem. We establish the first-order necessary condition of optimality from which optimal control can be obtained. The controlled states are calculated numerically and their linear stability is examined. We conclude that these states are strongly stable for situations of efficient reduction of enstrophy. In particular, we find that the pattern is substituted by a stable quasi conductive state.

Evolution equation for the subgrid heat fluxes in a finite-volume formulation. **Ivan Otic** (Forschungszentrum Karlsruhe, Germany) IC/CT4222/106

Large-eddy simulation (LES) of turbulent heat and mass transfer is a numerical approximation where the large scales of motion are supposed to be resolved while the small scales are modeled using a sub-grid scale (SGS) model. One approach for obtaining the SGS models consists in solving evolution equations for the sub-grid stress tensor and the sub-grid heat flux vector. This approach proposed by Deardorf and recently reinvestigated by Fureby, Tabor, Weller and Gosman may considerably improve the predictions at higher Reynolds numbers by minimal increase of computational cost. Definition of the large-scales to be simulated is similar to numerical discretization in that a finite-dimensional representation of an infinite dimensional solution is defined. The mapping to the finite dimensional representation (the filter) can be defined as in common numerical representations such as spectral, finite volume and finite element formulations. Clearly, the unrepresented sub-grid scales and the way they are modeled depend on the formulation used. Finite volume formulation is commonly applied because of its general applicability to flows in complex geometries.
We discuss here a finite volume formulation for a SGS heat flux model. We derive an evolution equation for the sub-grid heat flux vector for an LES filter that is consistent with finite volume representations. This derivation is similar to the derivations by Schumann and Grötzbach for the sub-grid kinetic energy and sub-grid temperature variance, respectively. The resulting equation has following properties:
1) it is consistent with Germano's filtering invariance property
2) there is a molecular term in the equation which does not appear in the equation derived by Deardorf.
This molecular term corresponds to the resolved scales of the heat flux dissipation rate and offers therefore an advantage for modeling and predictions of turbulent heat transfer. Using this equation we develop a differential sub-grid heat flux model. Algebraic SGS models seem to be very promising for engineering computations, as pointed out by Hanjalić. Assuming the small scale local equilibrium this evolution equation is simplified and an algebraic SGS heat flux model is derived.

10: Fluid Mechanics, Posters

IC/PP2254/010: **Parametric modulation in the Taylor–Couette ferro-fluid flow.**

Presenter: Jitender Singh (Punjab University, Chandigarh, India)
Co-author: Renu Bajaj (Punjab University, Chandigarh, India)

A parametric instability occurs in a dynamical system due to a modulation of some parameter. A Taylor-Couette system consisting of a viscous, incompressible flow of a Newtonian fluid in an annular region between to coaxial rotating cylinders is a good model to study this instabilty. Parametric instability in the viscous Taylor-Couette flow can appear by a time periodic oscillation of one or both the cylinders or a time periodic oscillation of the azimuthal velocity of the basic flow. The instability can also arise in the Taylor-Couette flow of a ferrofluid, via modulation of an axially applied periodically oscillating magnetic field to the system. We have investigated the response of the Couette-Taylor instability to the parametric modulation of a periodically oscillating magnetic field applied axially, using the classical Floquet theory.

IC/PP2032/101: **On the stability of forced KdV equation and forced modified KdV equation.**

Presenter: Jeongwhan Choi (Korea University, Republic of Korea)
Co-author: Sungim Whang (National Institute for Mathematical Sciences, Republic of Korea)

We derive both the time dependent Forced KdV and time dependent Forced Modified KdV equaion as model equations of a two layer incompressible immiscible and inviscid fluid over a small obstruction at the rigid bottom according to the variation of density ratio and depth ratio. By studying the equations both numerically and theoritically, we show the existence of the cut-off values of Froue number above which steady solution exist and below which no steady solution exist. The numerical stability of both Forced KdV equation and Forced Modified KdV equation are also carried out in this research.

IC/PP2613/101: **Geometrical effect of resonant gas oscillation excited in annular cavities.**

Presenter: Eru Kurihara (Hokkaido University, Japan)

The nonlinear resonance of cylindrical acoustic standing waves of an ideal gas contained between two coaxial cylinders is theoretically and numerically investigated. The wave motion concerned is excited by a small-amplitude harmonic oscillation of the radius of the outer cylinder, and the formulation of the problem includes the wave phenomenon in a hollow cylinder without the inner one as a limiting case. The spherical standing wave in two concentric spheres is also studied in parallel. The resonance occurs if the driving frequency falls in a narrow band around the linear resonance frequency, and in the weakly nonlinear regime, no shock wave is formed in contrast to the plane wave resonance. A cubic nonlinear equation for complex wave amplitude can then be derived by the method of multiple scales. Using a first integral of the cubic nonlinear equation, we shall demonstrate that the resonant oscillation is accompanied by a periodic modulation of amplitude and phase when the dissipation effect due to viscosity and thermal conductivity is negligible. The period of the modulation varies as the minus two-thirds power of the acoustic Mach number defined at the outer cylinder or sphere and decreases with an increase in the radius ratio of the inner and outer cylinders or spheres. When the dissipation effect is small but not negligible, the modulation is slowly weakened and the resonant oscillation approaches a steady state oscillation, which corresponds to the steady solution examined in earlier works. In the resonant oscillation generated between two eccentric cylinders, depending on the frequency of the sound source, axially symmetric or alternate oscillationg mode can be generated even if the sound source oscillates uniformly about the axis.

IC/PP4157/102: **Instability of uniformly-magnetized plasma and nonextensive theory.**

Presenter: Priyadarshi Patni (Jodhpur, India)
Co-author: Aiyub Khan (Jodhpur, India)

The dynamics of a self-gravitating, uniformly-magnetized plasma is studied in order to examine the propagation of hydromagnetic instabilities. The Jeans criterion is analyzed for modification due to nonextensive effects and the presence of an external magnetic field in the framework of Tsallis statistics. It is found that the Jeans instability is indeed modified by both these effects. A simple generalization of the Jeans criterion is derived.

IC/PP4706/103: **Analysis of the ice flow near the *grounding line*.**

Presenter: Ana Isabel Muñoz (Rey Juan Carlos University, E.S.C.E.T., Spain)

In this work we study one of the problems that has attracted more attention in the scientific community interested in the motion of glaciers, which is the *grounding-line* dynamics. The grounding line is the line where transition between ice attached to the solid ground and ice floating over the sea takes place. It is widely recognized that the ice flow behaviour in a neighborhood of the grounding line plays a very important role in the stability of the ice sheet. An example of this situation can be found in the West Antarctic Ice Sheet (W.A.I.S.).

We analyze a mathematical model describing the ice flow near the grounding line where the ice is considered a non-Newtonian fluid. To precise, we consider a stationary ice sheet modelled as a Stoke's flow in a bounded two-dimensional domain. The boundary that locates the interface ice–sea water is supposed to be unknown and determining its geometry and location is part of the problem. We prove the existence an uniqueness (in a sense to be defined) of weak solutions and find the regularity of the free boundary. We solve numerically the problem in a neighborhood of the grounding line, with a shooting method combined with an Euler one, in order to study locally the behavior of the velocity and stress fields. Finally, we present and discuss the numerical results for the problem in the whole domain, obtained with a finite-element method.

This is work done in collaboration with Marco A. Fontelos and Emanuele Schiavi.

IC/PP3051/106: **Riemann problem for a hyperbolic system of conservation laws in MHD.**

Presenter: Raja Sekhar Tungala (IIT Bombay, India)

We consider the Riemann problem for the system of equations which govern the one dimensional unsteady simple flow of an isentropic, inviscid and perfectly conducting compressible fluid, subjected to a transverse magnetic field . We show that system is hyperbolic, and establish existence of shocks and rarefaction waves. We prove the stability conditions for both the shocks and discuss how velocity and density vary across shocks and rarefaction waves. We show that the characteristic speed increases from left to right for rarefaction waves. We discuss properties of rarefaction curves and show that shock curves are starlike with respect to a some fixed point. We discuss the geometry of shock curves in Riemann invariant coordinates. We consider the Riemann problem for arbitrary initial data and show the existence and uniqueness of the solution under certain conditions. We discuss the vacuum state in isentropic magnetohydrodynamics. Finally we discuss the interaction of elementary waves obtained from the Riemann problem.

IC/PP805/106: **Mathematical simulations of flows in a tank containing an open elastic cylinder.**

Presenter: Lee Wanho (Wanho Lee, Republic of Korea)

Mathematical simulations of flows driven by pumping without valve was originally introduced by Jung using the immersed boundary method. Like many problems in biofluid mechanics, this can be modeled as the dynamic interaction of a viscous incompressible fluid (the blood) and elastic boundaries. In the present work, we consider a fluid filled tank with an open cylinder consisting a soft and rigid boundary. A periodic compression and decompression of the soft part generates a unidirectional flow. Both size and the direction of the generated net flow depend on the pumping frequency and amplitude.

11: Chemistry and Materials, Minisymposia

IC/MP80/011: **Multilinear decomposition: theory and applications.**

Organiser: Ilgis Ibragimov (Universität des Saarlandes, Germany)
Co-organiser: Vladislav Orekhov (Göteborg University, Sweden)

This minisymposium aims to bring together the world's leading researchers in multi-dimension and tensor decompositions.

The multi-dimension decomposition problem reads as following: let $f(x_1,\dots,x_d) \in \mathbb{C}$, with $x_1,\dots,x_d \in \Omega_d$, for given $d \in \mathbb{N}$ with $d > 2$. the aim is to find the rank-r decomposition through skeleton vectors $b_i^{(p)}(x_p)$, for $i = 1,\dots,r$ and $p = 1,\dots,d$, such that

$$f(x_1,\dots,x_d) \simeq \sum_{i=1}^{r} b_i^{(1)}(x_1)\dots b_i^{(d)}(x_d)\,.$$

Multi-dimension decomposition was first discussed in the works of Sokolov (1960) and Harshman (1971), but since that time it has still not been fully investigated. On the other hand, there is a strong interest to this decomposition in chemistry and physics. It is used for signal processing in telecommunications, optical and fluorescence spectroscopy, and in high-performance liquid chromatography. Another use[1] of this decomposition is for High-Resolution Multi-Dimensional NMR Spectroscopy, which makes a jump into the future for biochemistry.

[1] Jaravine, Ibragimov, Orekhov.; Removal of a TimeBarrier for High-Resolution Multi-Dimensional NMR Spectroscopy. Nature Methods. **3**, (2006) pp.605–607.

Optimization of resolution and sensitivity of NMR spectra using sparse matched data acquisition and multi-dimensional decomposition. **Vladislav Orekhov** (Göteborg University, Sweden) IC/MT2937/011

An overview of latest advances in the MDD methodology in the field of biomolecular NMR is presented. Reconstruction of a multidimensional spectrum from a non-uniformly sampled time signal is the equivalent to prediction of data lacking actual measurements. The mathematical model of the MDD assumes that all essential features of a M-dimensional matrix can be described as the sum of a small number of tensor products of one-dimensional vectors. When MDD is applied to NMR, the matrix corresponds to an input multidimensional time series, whereas the vectors represent output line-shapes. One of the merits of the original MDD method is that it does not apply any constraints on the appearance of the line-shapes. However, using a model with a smaller number of adjustable parameters has an advantage that a bigger fraction of missing data can be predicted. In most practical cases, the NMR theory predicts the autoregressive property of the time domain signal exemplified by a superposition of sine waves decaying with time.

We show that the autoregressive assumption can be incorporated into the MDD signal processing. In particular, each of the time domain shapes of length N in the original MDD model is recursively subjected to additional MDD decomposition to a product of K vectors of length d so that $N = dK$. This converts the original M-dimensional decomposition to $(M-1+K)$-dimensional one, which we entitle R-MDD. The aim of the second MDD decomposition is to reduce the number of unknowns in the least-square minimization in the MDD model. The original vectors with N unknown elements are defined by much smaller number of parameters $(d-1)\log_d(2N)$. The method allows to speed-up recording of high-resolution NMR spectra. In particular, logarithmic dependence on the dimension sizes and linear dependence on spectrum dimensionality essentially eliminates any practical restrictions on these parameters. For example, a $5D$ experiment with all indirect dimensions sizes of 100 points would take 101 years of measurement time using conventional uniform sampling scheme. R-MDD can sample such a spectrum in 2.4 hours, which is 13 times faster than offered by the original MDD processing. We demonstrate performance for several triple resonance experiments recorded on three globular proteins with molecular weights 8-22 kDa. For one of these systems good results are demonstrated with fraction of missing data of 94%, target spectra sizes of $400\times60\times100$ complex points, and number of spectral components 480.

This work was performed as a collaboration with V. Jaravine and I. Ibraghimov.

[1]. V. Orekhov, I. Ibraghimov, M. Billeter. Optimizing resolution in multidimensional NMR by three-way decomposition. *J. Biomol. NMR*, **2003**, 27(2): 165-173.

[2]. V. Tugarinov, L. Kay, I. Ibraghimov, V. Orekhov. High-resolution four-dimensional H-1-C-13 NOE spectroscopy using methyl-TROSY, sparse data acquisition, and multidimensional decomposition. *J. Am. Chem. Soc.*, **2005**, 127(8): 2767-2775.

[3]. V. Jaravine, I. Ibraghimov, V. Orekhov. Removal of time barrier for high-resolution multidimensional NMR spectroscopy. *Nature Methods*, **2006**, 3, 605-607.

Multi-dimensional decomposition of projected spectra obtained in protein NMR. **Martin Billeter** (Göteborg University, Sweden) IC/MT2776/011

Nuclear Magnetic Resonance (NMR) is a very versatile tool in protein research, e.g. for the development of clinically active compounds (*drug discovery*). The often several thousands signals in a NMR spectrum characterize structure, dynamics and interactions of proteins. These spectra are recorded as N-dimensional matrices with a few hundred data points along each dimension. Thus, conventional NMR experiments with $N \geq 5$ would yield matrices of excessive size (and require impossible measurement times). However, similar information to that of a spectrum with $N \sim 10$ is obtained by recording projections of such a spectrum. NMR theory describes the output of an N-dimensional experiment as

$$s(t_1,t_2\dots t_N) = \sum_k f_1(t_1)\otimes f_2(t_2)\dots\otimes f_N(t_N),$$

where t_i are time parameters of the experiment (called *evolution times*) and the functions f_i are of type $a\cdot\exp((i\omega-\lambda)\cdot t)$. The spectrum follows from Fourier transformation along all dimensions:

$$S(\omega_1,\omega_2,\dots,\omega_N) = \sum_k F_1(\omega_1)\otimes F_2(\omega_2),\dots,\otimes F_N(\omega_N)\,.$$

This equation describes a multidimensional decomposition with the experimental input on the left side and a characterization of the signals as the output on the right side. Projected spectra result from the coupling of evolution times: $t := c_1\cdot t_1 = c_2\cdot t_2,\dots = c_{N-1}\cdot t_{N-1}$. The projected spectrum becomes (after Fourier transform $t\to\omega, t_N\to\omega_N$)

$$S(\omega,\omega_N) = \sum_k (F_1\star F_2,\dots)(\omega)\otimes F_N(\omega_N)\,,$$

where $\star$ denotes convolutions. An implementation of an optimization procedure using the last equation to determine the functions F_i will be presented and applied to an experimental input of about 50 projected spectra with similar information content than a hypothetical 7-dimensional spectrum $S(\omega_1,\dots,\omega_7)$. The resulting F_i allow, using the second equation, reconstruction of parts of this spectrum $S(\omega_1,\dots,\omega_7)$, but they can also be directly interpreted to extract the desired signal information. Applications will be shown for protein molecules consisting of ~ 2500 atoms with the goal to identify their individual resonance frequencies.

Best rank-(R_1, R_2, R_3) approximation of third-order tensors, based on the Riemannian trust-region scheme. **Mariya Ishteva** (Katholieke Universiteit Leuven, Belgium), Lieven De Lathauwer (CNRS-ETIS, France), Pierre-Antoine Absil (Université Catholique de Louvain, Belgium), Rodolphe Sepulchre (Université de Liège, Belgium), Sabine Van Huffel (Katholieke Universiteit Leuven, Belgium) IC/MT1992/011

For matrices, the truncated Singular Value Decomposition (SVD) provides the best low-rank approximation. However, for tensors, the truncated Higher-Order SVD (HOSVD) [2], which is a generalization of SVD to higher-order tensors, gives a sub-optimal low-rank approximation, that can only be used as a starting value for iterative algorithms.

In this talk we propose an iterative algorithm for computing the best rank-(R_1, R_2, R_3) approximation of third-order (unstructured) tensors. We express the tensor approximation problem as minimizing a cost function on a manifold (a product of three Grassmann manifolds) and apply the Riemannian trust-region scheme [1], using the truncated conjugate-gradient method for solving the trust-region subproblem. Making use of second order information about the cost function, superlinear convergence is achieved. We present some simulation results.

[1] P.-A. Absil, C.G. Baker, K.A. Gallivan; Trust-region methods on Riemannian Manifolds. Accepted for publication in Found. Comput. Math., doi:10.1007/s10208-005-0179-9, 2006.
[2] L. De Lathauwer, B. De Moor, J. Vandewalle; A Multilinear Singular Value Decomposition. SIAM J. Matrix Anal. Appl., Vol. 21, No. 4, April 2000, pp.1253–1278.

IC/MP80/011: Multilinear decomposition: theory and applications. #2

Organiser: Ilgis Ibragimov (Universität des Saarlandes, Germany)
Co-organiser: Vladislav Orekhov (Göteborg University, Sweden)

(For abstract, see session #1 above.)

Multi-dimensional decomposition (MDD) of spontaneous electroencephalogramm (EEG). **Elena Orekhova** (Sahlgrenska University Hospital, Sweden) IC/MT3183/011

Electrical activity of the brain is essentially rhythmic. The functional coupling of a number of cortical brain regions is reflected by coherence or the rhythmic signals at corresponding EEG derivations. MDD is a powerful tool for analysis of complex multidimentional experimental data. We applied recursive MDD approach (Jaravine et al. Nature Methods 2006, 3: 605-607) to decompose EEG signal on a number of functional processes characterised by a frequency, phase and distribution over the head surface. In this study we used complex 10-12 dimensional decomposition with 2-20 components to deal with 2.7×10^5 complex data points. The calculations on simulated EEG signals were performed to evaluate potentials of the method for analysis of the real EEG. Preliminary results on EEG recorded during sustained visual attention in children are presented.

Solution of industrial linear systems with structured matrices. **Elena Ibragimova** (Elegant Mathematics Ltd., Germany) IC/MT3150/011

In this talk we present a "gray box" solver for large sparse linear system of equations and test it with different industrial problems. This solver utilize matrix entries and the grid where this matrix is generated.

If the system matrix uses a tensor grid, we use the Kronecker product approach, which can solve the system with linear and, in some cases, with sublinear complexity. In the case of general adaptive grids — a general sparse ILU preconditioners are used. The complexity and memory requirements of Kronecker product approaches are usually better than for the general ILU preconditioners. From the other hand, the adaptive grid without tensor structure can give better approximation of physical phenomena.

The main message of this talk is to compare an accuracy achieved in different grids using the best suitable approach for the solution of the linear system generated on several industrial problems. We present several numerical experiments and show that the answer to the question "which method is faster" is not evident for the most problems and it depends on many factors.

Problems in practical application of high-resolution numerical schemes to internal and external tasks of aerodynamics. **Egor Kazhan** (Central Aerohydrodynamic Institute, Russian Federation), Vladimir Vlasenko (Central Aerohydrodynamic Institute (TsAGI), Russian Federation), Sergey Bosniakov (Central Aerohydrodynamic Institute (TsAGI), Russian Federation), Sergey Glazkov (Central Aerohydrodynamic Institute (TsAGI), Russian Federation), Vladimir Jitenev (Central Aerohydrodynamic Institute (TsAGI), Russian Federation), Juergen Quest (European Transonic Windtunnel, Germany), Sergey Mikhailov (Central Aerohydrodynamic Institute (TsAGI), Russian Federation) IC/MT2618/011

This report presents numerical method for solution of aerodynamic tasks on the basis of Reynolds Averaged Navier-Stokes Equations. The method is applied to simulation of flow around aircraft (including engine-airframe interference) and to description of flowfield in the wind tunnel (WT) with aircraft model inside. Because of growing practical requirements both to accuracy of numerical results and to calculation time, further improvement of numerical methods is necessary. Possible way is optimal combination of explicit and implicit schemes. Advantages of explicit schemes - small cost per one time step and relatively small errors in simulation of unsteady processes. But strong time step restriction leads to huge computation times in tasks with vastly different linear scales. Implicit schemes may be stable for each value of time step. But they produce high errors in description of unsteady processes and high cost per time step. We recommend zonal approach: flow regions with small scales of physical phenomena may be described using implicit scheme, and the rest of the flowfield - using explicit scheme. Further in the report, examples of the existing numerical method application to practical tasks of aerodynamics are presented. Numerical calculations may be used at various stages of experiment preparation: they aid to choose the placement of gauges, to avoid errors during tests, to interpret the obtained data, to adjust WT wall perforation and to eliminate errors caused by WT walls influence on the model. An example of modeling flow in the test section of European Transonic Windtunnel is shown. Unsteady phenomena around WT slotted walls were obtained.Calculations of noise suppressing nozzles with different geometry are considered. Numerical simulation has allowed to improve the nozzle geometry and to provide essential noise suppression. All presented examples confirm the need in further development of effective and accurate algorithms for practical tasks solution.

Fast numerical solution of Boltzmann equation. **Ilgis Ibragimov** (Universität des Saarlandes, Germany) IC/MT3090/011

This talk consider a fast numerical solution of the classical Boltzmann equation for a simple, dilute gas of particles:

$$f_t + (v, \nabla_x f) = \int_{\mathbb{R}^3} \int_{S^2} B(v, w, e)(f(v')f(w') - f(v)f(w))\mathrm{d}e\mathrm{d}w\,,$$

where

$$f(t, x, v) : \mathbb{R}_+ \times \Omega \times \mathbb{R}^3 \to \mathbb{R}_+$$

describes the time evolution of the particle density.
It is observed that the particle density function can be considered as low multi-dimensional rank function and reads in the form

$$f(t, x, v) = \sum_{i_1, i_2, i_3}^{r_1, r_2, r_3} f_{i_1}^{(1)}(t, v_1, x) f_{i_2}^{(2)}(t, v_2, x) f_{i_3}^{(3)}(t, v_3, x) g_{i_1, i_2, i_3},$$

where r_1, r_2, r_3 are almost constants.

This approach needs $\mathrm{O}(n)$ words of memory for each grid points of domain discretisation, which is comparable to descretisation of Navier–Stokes equations, but produce better numerical accuracy. Here n denotes the number of discretisation points in one direction of the velocity space.

The method has been tested on an industrial example of supersonic flight simulation with Mach number > 10, having 1.2 million grid points in the domain Ω, and $n = 64$. The simulation takes several days using a modern PC. To obtain a similar result by other deterministic methods one should use a supercomputer having terabytes of main memory.

IC/MP192/015: Mathematical models for cultural heritage.

Organiser: Roberto Natalini (Consiglio Nazionale delle Ricerche, Italy)
Co-organiser: Antonio Fasano (Università di Firenze, Italy)

The minisymposium aims to present some current researches about the rational assessment and quantitative prediction of damage in cultural heritage, with a specific focus on surface and structural damage in natural stones and concretes used in historical buildings or artifacts, through a systematic use of mathematical models. The presentations will be concerned with phenomena occurring under the combined attack of different aggressive agents like pollution, weathering, moisture, vibrations, and thermal variations.

Free-boundary models of sulphation: swelling and the influence of humidity. **Fabrizio Clarelli** (Consiglio Nazionale delle Ricerche, Italy), Antonio Fasano (Università di Firenze, Italy), Roberto Natalini (Consiglio Nazionale delle Ricerche, Italy) IC/MT1412/015

Deterioration of stones is a complex problem and one of the main concern for people working in the field of conservation and restoration of cultural heritage. It is extremely difficult to isolate a single factor in this kind of processes, which are the results of the interaction of various mechanisms, many of which also occur in natural weathering, even is atmospheric pollution can be considered as one of the most important factor of damage. Here, we introduce some free boundary models which describe the evolution of calcium carbonate stones under the attack of atmospheric SO_2, taking into account both swelling of the external gypsum layer and the influence of humidity. Different behaviors are described according to the relative humidity of the environment, and in all cases reliable explicit asymptotic approximations are introduced under reasonable assumptions on the data. Numerical simulations are introduced and discussed.

Fracture of concrete due to corrosion. **Yves Berthaud** (Université Pierre et Marie Curie, France), Caré Caré (Laboratoire Central des Ponts et Chaussées, France), Ragueneau Ragueneau (LMT Cachan, France), Thanh Thanh (LMT Cachan, France), Millard Millard (Commissariat à l'Energie atomique, France), L'Hostis (Commissariat à l'Energie atomique, France) IC/MT1817/015

Cracking of concrete due to corrosion is a very common pathology that can be observed on various structures. Corrosion is initiated by the penetration of chlorides or of carbon dioxide in most cases. The consequences of corrosions are (i) the reduction of the resistive section of reinforcements (ii) the creation of expansive products (commonly denoted rust) (iii) the fragilization of steel and finally (iv) the cracking of concrete. Three stages are distinguished: (1) the incubation that corresponds to diffusion processes of chemical species (ions) inside concrete from the free surface to the steel concrete interface ; (2) the initiation stage starts when the passivation film is broken ; (3) the cracking stage corresponds to the end of the initiation and to the lack of carrying capacity of the structure. We have decided to study this stage in Laboratory. The first stage takes decades for real cases. In our study it has been speeded by the use of accelerated corrosion under the effect of imposed electrical current with the addition of chorides in the mixture (they act as a catalyser for the chemical reaction). We decided to impose the electrical current density that allows to predict (using the FaradayŠs law) the production of iron oxides. The imposed values range between 1 and $5A/m^2$. We have designed various types of specimens for plane strain and plane stress analyses. They give us the possibility to record digital images that are analysed through the LMT-soft Correli ; it computes both the in plane displacement and the plane strain fields. It is possible to derive the kinetics of damage that has been proved to be similar to what happens in real structures (for natural corrosion). A finite element modelling has been developed based on a classical damage model for concrete, on the identified properties of iron oxides (very low stiffness) and on the use of special interface elements. The growth of oxyde layer is obtained via an imposed fictitious thermal load the rate of which is calibrated to fit real data (measured using long distance microscope).

Progress and challenges in modelling salt damage to building stones. **Heather Viles** (University of Oxford, UK) IC/MT2677/015

Much important built heritage worldwide is composed of porous building stones, and many of these stones are at risk of damage from salt crystallisation. Salts may enter porous stone dissolved in groundwater or precipitation, and come from sources as diverse as air pollution, deicing salts, dust and natural weathering. Damage to stonework occurs when salts within pores repeatedly crystallise, dissolve and recrystallise, exerting pressures on the pore walls which eventually result in failure (often in the form of crack propagation and spalling). There has been a long history of field and laboratory-based studies on salt crystallisation, and more recently a variety of attempts have been made to model the processes at work. We review some recent models which have focused either on what happens in single pores or on the larger scale development of decay features such as alveoli. We suggest some potentially valuable new approaches to the problem, with a view to providing a more complete model of how salt crystallisation causes damage to stonework.

Wetting of rough surfaces. **Antonio DeSimone** (SISSA, Trieste, Italy) IC/MT3905/015

We discuss wetting properties of chemically or topographically patterned surfaces. In particular, we analyze the effect of roughness on the apparent contact angle and contact angle hysteresis through a variational approach and homogenization techniques. Perspectives for the analysis of graffiti damage and antigraffiti measures for monuments and buildings will be discussed. This is joint work with G. Alberti, N. Grunewald, and F. Otto.

IC/MP999/110: Electronic structure calculation.

Organiser: Reinhold Schneider (Universität Kiel, Germany)

The electronic Schrödinger equation describes the non-relativistic behaviour of a quantum mechanical N-electron system under the influence of Coulombic potentials. It is the basic equation for ab initio numerical simulation of phenomena on an atomic or molecular scale. Density functional theory provide effective one particle models to circumvent the approximation of the wave function in high dimensions. Approaches which scale linearly with respect to the number of atoms could provide tools for computing extremely large molecules or atomic clusters up to the systematic error of the underlying DFT model. The approximation of the high dimensional wave function is extremely difficult, Recent regularity and approximation results indicate that the wave functions can be approximated with a polynomial instead of an exponential scaling w.r.t. to the number of particles. Highly accurate computational results for the correlation energy are achieved by the coupled cluster method, frequently used in quantum chemistry.

Convergence of the coupled-cluster method. **Reinhold Schneider** (Universität Kiel, Germany) IC/MT3748/110

The coupled cluster (CC) method is known to provide a powerful approach for the numerical computation of correlation energies if dynamic correlation effects are dominating. It provides an approximation of the solution of the electronic Schrödinger equation. The convergence behaviour of the projected coupled cluster method (brievely called coupled cluster method) is considered. This method is introduced as an approximation of the full CI solution. Error estimates for the energies are shown by a Aubin Nitsche type arguments using the dual weighted resiual approach.

Towards an a posteriori *error representation to the Hartree–Fock equations.* **Stephan Schwinger** (Max-Planck-Institut Leipzig, Germany) IC/MT3752/110

The Hartree-Fock equations are of basic interest in *ab initio* quantum chemistry. They constitute a nonlinear eigenvalue problem, which has to be solved numerically. This means one has to select an efficient basis for discretizing this problem. In the chemical community, the approximation error commited thereby has hardly been analysed. In the last decade, *a posteriori* error estimation has grown an important tool for the determination of the approximation space for partial differential equations. Often, one is not interested in the error of the approximate solution with respect to some global norm, but rather to improve the error in the value of some target functional computed from it. This is the aim of the so-called Dual Weighted Residual Method, which we want to apply to the Hartree-Fock equations.

Fast wavelet-based methods for electrostatic and quantum mechanical problems. **Stefan Goedecker** (Universität Basel, Switzerland) IC/MT3899/110

Electronic structure calculations require to solve Poisson's and Schrödinger's equations. First, a family of methods will be presented that allows to solve electrostatic problems for both continous and discrete charge distributions with $N\log(N)$ scaling under various boundary conditions. These methods are thus an alternative to fast multipole, particle mesh and plane wave methods. Second, it will be shown how Daubechies' wavelets can efficiently be used as a basis set for pseudo-potential density functional calculations.

Sparse grids, adaptivity, and symmetry. **Andreas Zeiser** (TU Berlin, Germany), Harry Yserentant (TU Berlin, Germany) IC/MT3915/110

Sparse grid methods represent a powerful and efficient technique for the representation and approximation of functions and particularly the solutions of partial differential equations in moderately high space dimensions. To extend the approach to truly high-dimensional problems as they arise in quantum chemistry, an additional property has to be brought into play, the symmetry or antisymmetry of the functions sought there. In the talk, an adaptive sparse grid refinement scheme is presented that takes full advantage of such symmetry properties and for which the amount of work and storage remains strictly proportional to the number of degrees of freedom. To overcome the problems with the approximation of the inherently complex antisymmetric functions, augmented sparse grid spaces are proposed.

IC/MP30/111: Kinetic Monte-Carlo methods.

Organiser: Tim Schulze (University of Tennessee, USA)
Co-organiser: Shaun Hendy (Industrial Research Ltd, New Zealand)

Kinetic Monte Carlo (KMC) is a stochastic simulation technique widely used to study epitaxial growth, chemical kinetics and other discrete stochastic processes. With its growing popularity, a large number of novel techniques and algorithmic improvements are emerging. The minisymposium will cover a range of these emerging methods, including hybrid simulation techiques, self-learning and adaptive KMC, off-lattice KMC, parallel implementation and fast algorithms.

Rare events in kinetic Monte-Carlo. **Eric Vanden-Eijnden** (Courant Institute, NYU, USA) IC/MT958/111

In this talk, rare events in the context of continuous-time Markov jump processes and networks will be discussed. In particular, it will be shown how Freidlin-Wentzell theory of large deviations can be used to design an efficient numerical technique, termed the minimum action method, to determine the pathways of maximum likelihood of hopping events between metastable basins as well as the rate of occurence of these events. The method will be illustrated on some chemical and biological networks.

Efficient computation of heteroepitaxial growth. **Peter Smereka** (University of Michigan, Ann Arbor, USA) IC/MT1168/111

The growth of strained heteroepitaxial films using a Solid-on-Solid model KMC is discussed. Elastic effects are included by using a ball and spring model. Discrete models of this form naturally include nanoscale effects, such as nucleation, which are difficult to incorporate in continuum models. On the other hand, it is more computationally intensive to use these discrete models to simulate film growth on experimentally relevant length scales. This talk will discuss some of the computational challenges and approaches we have developed for simulation of heteroepitaxy. In particular, I will discuss a multigrid-Fourier method for rapid solution of the displacement field, an expand box method which allows very quick local corrections to the displacement field, and a rejection-reduced KMC method which uses fast estimates of the hopping rates. Preliminary results of film growth will be presented which shows that when the elastic effects are small the film grows in a layer-by-layer fashion. However, when the elastic effects become strong we observe strain relaxed three dimensional islands sometimes called self-assembled quantum dots.. This is joint work with Giovanni Russo and Tim Schulze.

A hybrid kinetic Monte-Carlo molecular dynamics method for modeling epitaxial growth. **Shaun Hendy** (Industrial Research Ltd, New Zealand), Tim Schulze (University of Tennessee, USA), Peter Zoontjens (Victoria University of Wellington, New Zealand) IC/MT1235/111

The disparate time and length scales involved in the epitaxial growth of thin films pose an enormous challenge for simulation. A popular and powerful approach to the simulation of such processes is the kinetic Monte Carlo (KMC) method, especially when combined with first principles determinations of rates. While the standard KMC method assumes that atoms reside on a perfect lattice, this approximation is not always appropriate. For instance, growth on a fcc (111) surface can lead to the formation of both fcc and hcp islands, and the subsequent the formation of grain boundaries as these islands impinge. While the mobility of grain boundaries is an important factor in determining the quality of thin films, this may be poorly described by the usual lattice approximation favored by standard KMC. Molecular dynamics (MD) on the other hand does not rely on a lattice approximation. With an appropriate potential energy function, one would expect MD to give an accurate description of the structure and dynamics of a grain boundary. However, MD can only be used to simulate a relatively small number of atoms for relatively short durations due to the need to compute forces between pairs of atoms on time scales much smaller than those generally involved in KMC. This generally prohibits the use of MD in simulating epitaxial growth except in the limits of high temperatures and high deposition rates. Here we present a hybrid multiscale method which combines MD and KMC in a spatial domain decomposition in an attempt to speed up conventional MD. Near the grain boundaries, atoms are treated using MD but away from the boundaries we use KMC. We apply this method to study the motion of grain boundaries during epitaxial growth.

IC/MP30/111: Kinetic Monte-Carlo methods. #2

Organiser: Tim Schulze (University of Tennessee, USA)
Co-organiser: Shaun Hendy (Industrial Research Ltd, New Zealand)

(For abstract, see session #1 above.)

Fast kinetic Monte-Carlo algorithms. **Tim Schulze** (University of Tennessee, USA) IC/MT2035/111

Two new algorithms for KMC simulations designed to give a fixed single-event execution time as the system size is increased will be described. These algoithms address systems with large event lists and disparate rates that do not cluster at a small set of discrete values. The methods will be demonstrated using models for crystal growth.

Numerical analysis of coarse-graining in stochastic simulations. **Petr Plecháč** (Univ. Tennessee & Oak Ridge National Lab, USA) IC/MT2718/111

We shall discuss some general mathematical and numerical issues arising in simulations where the microscopic Markov process is approximated by a hierarchy of coarse-grained processes. We shall present mathematical tools (e.g., entropy estimates estimates) for error estimation of the coarse-graining procedure. The techniques will be explained in specific examples of lattice as well as off-lattice dynamics and various types of error control will be presented. Analysis of convergence to equilibrium will be also discussed. Numerical evidence supported with rigorous analysis indicates regimes in which the coarse-grained Monte Carlo algorithm probes efficiently energy landscape and provides accurate approximation of sampled quantities.

Self-learning kinetic Monte-Carlo simulations: application to epitaxial growth processes. **Talat Rahman** (University of Central Florida, USA) IC/MT3789/111

Coupled with advances in ab initio methods for the calculation of activation energy barriers, the kinetic Monte Carlo (KMC) method is proving itself to be an important tool for computational studies of phenomena such as epitaxial growth, surface diffusion and surface morphological evolution. However, despite its ability to carry out simulations for time and length scales that are relevant to experiments, in its nascent form the method has limited predictive power because of its reliance on predetermined atomic events and their energetic as input. To overcome this handicap, we have developed a self learning method (SLKMC) within the lattice gas model, in which we combine standard KMC with automatic generation of a table of microscopic events, facilitated by a pattern recognition scheme. Each time the system encounters a new configuration, the algorithm initiates a procedure for saddle point search around a given energy minimum. Nontrivial paths are thus selected and the fully characterized transition path is permanently recorded in a database for future usage. The system thus automatically builds up all possible single and multiple atom processes that it needs for a sustained simulation. Results of the application of the method to examination of the diffusion and coalescence of 2-dimensional Cu and Ag adatom and vacancy clusters on Cu(111) and Ag(111) will be presented. I will highlight the key role played by specific diffusion processes revealed during the simulation. Of particularly interest are multiple atom processes whose presence may have been ignored otherwise. As we will see the importance of such processes is dependent on both cluster size and surface temperature. For adatom clusters varying in size from 2 to 1000, I will discuss the size dependence of the diffusion coefficient and the effective energy barrier. The rate limiting processes will also be discussed for island coalescence. Results will be compared with those from experiments, where available, and with those from KMC simulations based on a fixed catalogue of diffusion processes. I will also provide some details of an extension of the techniques to Şoff-latticeŤ case and its application to examine the case of heteroepitaxial growth.

1Work done in collaboartion with A. Kara, A. Karim, A. Al-Rawi, and O. Trushin *Work supported in part by NSF and CRDF

IC/MP286/112: Recent development in the mathematical theory of polymeric materials: modeling, numerical simulation, and analysis.

Organiser: Bo Su (Iowa State University, USA)
Co-organiser: Vincenzo Capasso (Università degli Studi di Milano, Italy)

This minisymposium is to provide a forum to foster research exchange and collaboration among active reseachers in the area who are addressing the fundamental problems from crystal growth, crystal nucleation, polymer nanocomposite to polymeric fluid.

Random geometric birth-and-growth processes in material sciences and biomedicine. **Vincenzo Capasso** (Università degli Studi di Milano, Italy) IC/MT3377/112

Nucleation and growth processes arise in a variety of natural and technological applications, such as solidification of materials, semiconductor crystal growth, biomineralization (shell growth), tumour growth, vasculogenesis, etc. All these processes may be modelled as birth-and-growth processes (germ–grain models), which are composed of two processes, birth (nucleation, branching, etc.) and subsequent growth of spatial structures (crystals, vessel networks, etc), which, in general, are both stochastic in time and space. These structures usually induce a random division of the relevant spatial region, known as a random tessellation. A quantitative description of the spatial structure of a random tessellation can be given, in terms of the mean densities of interfaces (n-facets) of the random tessellation, at different Hausdorff dimensions (cells, faces, edges, vertices), with respect to the usual d-dimensional Lebesgue measure. In Material Science mechanical properties of the final material strongly depend on the mean densities of the interfaces. Predictive mathematical models which are capable of producing quantitative morphological features can contribute to the solution of optimization or optimal control problems. A non-trivial difficulty arises from the strong coupling of the kinetic parameters of the relevant birth-and-growth (or branching-and-growth) process with the underlying field, such as temperature, and the geometric spatial densities of the evolving spatial random tessellation itself. Methods for reducing complexity include homogenization at mesoscales, thus leading to hybrid models (deterministic at the larger scale, and stochastic at lower scales).

Ginzburg–Landau minimizers with prescribed degrees: emergence of vortices and existence/nonexistence of the minimizers. **Leonid Berlyand** (Pennsylvania State University, USA) IC/MT1475/112

Let Ω be a 2D domain with a hole ω. In the domain $A = \Omega \setminus \omega$ consider a class $\mathcal{J}$ of complex-valued maps having degrees 1 and 1 on $\partial\Omega$, $\partial\omega$ respectively.

In a joint work with P. Mironescu we show that if $\mathrm{cap}(A) \geq \pi$ (subcritical domain), minimizers of the Ginzburg-Landau energy E_κ exist for each κ. They are vortexless and converge in $H^1(A)$ to a minimizing S^1-valued harmonic map as the coherency length κ^{-1} tends to 0. When $\mathrm{cap}(A) < \pi$ (supercritical domain), for large κ, we establish that the minimizing sequences/minimizers develop exactly two vortices—a vortex of degree 1 near $\partial\Omega$ and a vortex of degree -1 near $\partial\Omega$ which rapidly converge to ∂A. It was conjectured that the global minimizers do not exist for large κ.

In a subsequent joint work with D. Golovaty and V. Rybalko this conjecture was proved. It was shown that, when $\mathrm{cap}(A) < \pi$, there exists a finite threshold value κ_1 of the Ginzburg–Landau parameter such that the minimum of E_κ is not attained in $\mathcal{J}$ when $\kappa > \kappa_1$, while it is attained when $\kappa > \kappa_1$. No standard elliptic estimates worked here and our proof is based on an introduction of an auxiliary linear problem which allows for an explicit energy estimate which is sufficiently tight.

Ginzburg–Landau equations with two order parameters. **Daniel Phillips** (Purdue University, USA) IC/MT3334/112

We study a G-L model for high-T_c superconductivity described with two complex valued order parameters; a dominant d-wave component and a small admixture of an s-wave component. In this model, if the s-d mixing parameter is zero then the system reduces to the standard single component G-L equation. We investigate the case of a small mixing parameter and the nucleation of the second component. This is joint work with Minkyun Kim.

Modelling Ziegler–Natta polymerization in high-pressure reactors. **Alberto Mancini** (Università di Firenze, Italy), Antonio Fasano (Università di Firenze, Italy) IC/MT601/112

The Ziegler–Natta process in its modern version, using spherical catalyst support in high-pressure reactors, is the most efficient and economic way of producing polymers of ubiquitous use such as polypropylene and polyethylene. Using the ideas of previous works as a starting point, we present a mathematical model encompassing for the first time the mechanical behavior of the polymer while it grows around the nanometric catalytic particles. As a theoretical basis for the description of the growing continuum we use the theory of *Natural Configurations* of K.R. Rajagopal and L. Tao.

IC/MP286/112: Recent development in the mathematical theory of polymeric materials: modeling, numerical simulation, and analysis. #2

Organiser: Bo Su (Iowa State University, USA)
Co-organiser: Vincenzo Capasso (Università degli Studi di Milano, Italy)

(For abstract, see session #1 above.)

Interfacial flows with surfactant. **John Lowengrub** (University of California, Irvine, USA) IC/MT3244/112

In this talk, I will present Eulerian methods for the simulation of fluid interfaces with surfactant using a level-set method. The methods couple an implicit discretization of the surfactant equation with the immersed interface flow-solver. Novel techniques are used to accurately conserve component mass and surfactant mass during the evolution. The method is applied to study the effects of surfactants on single drops, drop-drop interactions and interactions among multiple drops in Stokes flow under an applied shear. A non-monotonic behavior of the minimum distance between approaching drops versus capillary number is observed. Accordingly, a critical capillary number Ca* measuring the tendency to coalescence is determined as a function of the surfactant coverage. A transition in behavior is observed to occur at a critical coverage. This is joint work with J. Xu, Z. Li and H.-K. Zhao.

Direct and inverse modeling for stochastic data in microbead rheology with application to biological liquids. **Christel Hohenegger** (University of North Carolina, USA) IC/MT5060/112

The need in biology to understand the rheological properties of cells, tissues, membranes, and biological liquids, has led to new techniques in microrheology, where bead tracking is the fundamental probe of viscoelastic properties. We present stochastic methods for inverse characterization based on noisy time series, starting with the Mason-Weitz protocol for single bead path data, then going to the Crocker-Levine-Lubensky protocol for 2-point statistics. We build fast and statistically accurate direct simulation tools based on generalized Langevin equations, as well as inversion methods derived from maximum likelihood methodology and Kalman filter. The motivating application is to support experiments by R. Superfine and D. Hill and for characterization and simulations of transport mechanisms in lung airway surface liquids within the Virtual Lung Project at UNC Chapel Hill.

Inhomogeneous kinetic theory of liquid-crystal polymers. **Pingwen Zhang** (Peking University, PR China) IC/MT1525/112

We study the microstructure formation and defects dynamics arising in liquid crystalline polymers by a coupled kinetic-hydrodynamic multi-scale model. The kinetic model is an extension of Doi theory with a non-local intermolecular potential, including translational diffusion and density variation. LCP molecules were ensured anchoring at the boundary by an additional boundary potential, meanwhile mass conservation of LCPs holds in the whole flow region.

Plane Couette flow and pressure-driven Poiseuille flow are studied using the kinetic-hydrodynamic model. In plane Couette flow, the numerical results show that: 1) not only all of four in-plane modes reported by Rey and Tsuji [Macromol. Theory Simul. **7** (1998) 623–639] but also complicated in-plane modes with multi-layer defects were found; 2) some significant scaling properties were verified, such as the thickness of boundary layer is proportional to the ratio of molecular length to the size of the flow region, the tumbling period is constant in dimensionless time and has little relation with dimensionless parameters, and so on. In pressure-driven plane Poiseuille flow, the micro-morph is quasi-periodic in time when flow viscosity and molecular elasticity are comparable. Different states, such as flow-aligning, tumbling or wagging, arise in different flow region. The difference of the tumbling rate in near-by regions causes defects and form branch pattern in director spatial-temporal configuration figure.

Moment closure for FENE models of complex fluids. **Qiang Du** (Pennsylvania State University, USA) IC/MT1963/112

Moment closure not only provides a computationally feasible approach to simulate many multiscale phenomena but also offers insight to the understanding of the underlying physical processes. We will discuss some of our recent works on developing systematic moment closure models for micro-macro FENE models of complex fluids and demonstrate their effectiveness for a wide range of parameter regimes. This is a joint work with colleagues at Penn State: C. Liu, P. Yu and Y. Hyon.

11: Chemistry and Materials, Contributed Talks

IC/CTS4900/11: **Chemistry and materials.**

Organiser: Alexander Zhmakin (St.Petersburg Branch of Joint Supercomputer Center, Russian Federation)

Relating atomistic-to-continuum coupling and domain decomposition. **Michael Parks** (Sandia National Laboratories, USA), Pavel Bochev (Sandia National Laboratories, USA), Richard Lehoucq (Sandia National Laboratories, USA) IC/CT1316/111

The deformation and failure of many engineering materials are inherently multiscale processes. Models for such processes frequently call for decomposition of the material domain into atomistic and continuum subdomains, where the continuum subdomain is modeled via a finite element analysis. The treatment of the boundary between these subdomains, or "handshake region", is frequently what distinguishes one atomistic-to-continuum coupling method from another. A formal theory of this transition region does not yet exist. Instead, current coupling schemes employ ad hoc approximations, such as treating finite element nodes as atoms, or vice-versa, to accommodate the incompatibility between a non-local atomistic description and a local finite element description at the atomistic/continuum boundary. There currently exists little rigorous analysis of these schemes.

The atomistic-to-continuum coupling problem has similarities with the classical continuum-to-continuum domain decomposition problem. We will explore some of these similarities and address the extent to which both problems can be placed within the same mathematical and algorithmic framework. We will address domain decomposition methods that can be harnessed when solving the atomistic-to-continuum coupling problem, and for a particular coupling scheme, provide a convergence theory giving guidance about when the scheme will produce a satisfactory answer.

Modelling competition assays for electrochemical biosensors. **Dana Mackey** (Dublin Institute of Technology, Ireland), Anthony Killard (Dublin City University, Ireland) IC/CT3076/015

Biosensors are devices in constant development due to their wide use in biomedical diagnostics and environmental monitoring. Of particular interest to developing electrochemical immunosensors are enzyme channelling systems, where two enzymes are brought in close proximity to an electrode surface thus facilitating the fast conversion of initial substrate to final product.

This study compares the behaviour of an electrochemical bi-enzyme biosensor with a theoretical analysis based on a mathematical model, consisting of reaction-diffusion equations with nonlinear boundary conditions, and numerical simulations. The model describes transport processes and chemical reactions taking place in the bulk solution and at an electrode boundary, and focusses on the competition between a given antigen and its enzyme-labelled analogue for binding to electrode-immobilised antibodies. Problems of practical significance, such as determining optimal values for system design parameters with the aim of maximising the amperometric signal amplitude, while keeping non-specific interactions to a minimum, are also addressed.

Step-flow growth with anomalous diffusion. **Margo Levine** (Northwestern University, USA), Alexander Golovin (Northwestern University, USA) IC/CT2562/015

The growth of a stepped crystal surface by molecular beam epitaxy is investigated in the case when the adatom diffusion is anomalous (super-diffusion). The analog of the Burton–Cabrera–Frank theory for the case of super-diffusion is developed. The step-flow velocity is obtained as an eigenvalue of the corresponding super-diffusion problem described by a fractional PDE. The resulting crystal surface growth rate is found as a function of the terrace length and the anomalous diffusion exponent. The linear stability analysis of the step shape is performed and the super-diffusion analog of the Bales–Zangwill instability caused by the Schwobel effect is studied.

Numerical study of facetted dielectric crystal growth. **Alexander Zhmakin** (St.Petersburg Branch of Joint Supercomputer Center, Russian Federation) IC/CT3140/011

The aim of the paper is to numerically study processes at the melt/crystal interface during the growth of dielectric crystals under the action of either an intentionally introduced impurity or a local heating by a laser irradiation and to asses the effects of such interventions on the growth stability and behaviour of macrosteps on the crystal surface. The growth regimes where the undercooling of the facetted crystallization front is significant are considered.

Local computations are coupled to the global heat transfer in the whole crystal growth facility.

Computations are supported by experimental investigation of growth of bismuth germanate crystals by the crucibless AHP method.

Work done in collaboration with V.D. Golyshev.

Numerical methods for the chemical master equation and applications to stochastic models or receptor oligomerisation. **Shev Mac** (University of Queensland, Australia) IC/CT2046/015

The chemical master equation is an important model for studying chemical kinetics, especially in the context of systems biology where noise is known to play an important role and so a discrete and stochastic framework is required. However due to the high dimensional nature of the equations it has often been felt to be too difficult to tackle numerically, although recently much progress has been made. Here some novel numerical methods are presented and applied to stochastic models of receptor oligomerisation, which have previously been studied only by simulation. This gives a novel perspective on these models and suggests some insights into the phenomena of the role they play in buffering cell signals.

11: Chemistry and Materials, Posters

IC/PP2672/015: **The semi-empirical relaxation operator in quantum Liouville equation and computer simulation of two-spin system magnetic resonance spectra.**

Presenter: Vladimir Privezentsev (Institute of Physics and Technology RAS, Russian Federation)

In present work the structure of the semi-empirical relaxation operator in Liouville quantum equation was carried out. This equation for the magnetic transition M is used at computer simulation magnetic resonance spectra of a two-spin system [1]. An introduction of this phenomenological operator allows us to expand application of Liuville quantum equation to nonequilibrium processes. There are absorption by two-spin system of the superfluous μ-wave quantums and interaction of the two-spin system with environment spin medium. For the calculation of such magnetic resonance spectra a perturbation theory is not used [2].

Liouville quantum equation is written in matrix form as $\dot{M}_{mn} = \sum_{j,k} L_{mjkn}\left(M_{jk} - M_{mn}\right) + M_{mn}\sum_{j,k} L_{mjkn}$, in which $L_{mjkn} = iH_{mj}\delta_{kn} - i\delta_{mj}H_{kn}$. Here, H_{mn} is a matrix element of the spin Hamiltonian and δ_{mn} is the Kronecker delta, $\delta_{mn} = 1$ for $m = n$, and $\delta_{mn} = 0$ for $m \neq n$. To evaluate the relaxation components, we assume [3] that, due to relaxation, Liouville quantum equation describes a complete chain of equations, the transition rate ν_{mn} between the spin states ψ_m and ψ_n being a function of the imaginary quantities iH_{mn} and $-iH_{mn}$. We suppose also, that the component representation of the relaxation operator is structurally similar to that of the Liouville operator, with real ν_{mn} substituted for $\pm iH_{mn}$. We change likewise from δ_{mn} to the overlap functions p_{mn} in order to allow for the stochastic interaction of the paramagnetic center with its surroundings $\langle\psi_m\psi_n\rangle = p_{mn}$ which is < 1, for $n = m$ or > 0 for $n \neq m$. It should be clear, that $\nu_{mn} \to 0$ and $p_{mn} \to \delta_{mn}$ as the density of active surrounding active spin particles decreases. Thus, the semiempirical relaxation operator is four-index relaxation matrix with real members: $R_{mjkn} = \nu_{mj}p_{kn} + p_{mj}\nu_{kn}$.

This is work done in collaboration with Dobryakov, Sergey. Semenov Institute of chemical physics, Russian Academy of Science, ul. Kosygina, 6, 117799 Moscow, Russia.

[1] Dobryakov, S.N.; in *Bioactive Spin Labels* (ed. by Zhdanov, R.I.). Springer-Verlag, Berlin, 1992, p.215.

[2] Dobryakov, S.N. and Privezentsev, V.V.; Computed Equilibrium ESR Spectra of the $P\,{}^{-28}Si - \ldots {}^{-28}Si - P$ Structure for a Spin Register. Obozr. Prikl. Prom. Matem. v.12, No. 3, p.576 (2005) (in Russian).

[3] Dobryakov, S.N., Privezentsev, V.V.; Mathematical modeling and computer simulation of a two-spin system magnetic resonance spectra. Intern. Congr. of mathemat., Abstr. Post., Short Comm. et al, p.140, Madrid (2006).

IC/PP2888/110: **Monte-Carlo study of transition temperature of Mn-doped GaN diluted magnetic semiconductor.**

Presenter: Jeffrey Rufinus (Widener University, USA)

We have used a large scale Monte Carlo simulation technique to study the effect of metal cluster distribution on the transition temperature of Mn-doped GaN Diluted Magnetic Semiconductors. To calculate the transition temperature via Monte Carlo simulations, a Density functional theory (DFT)-based Locally Self Consistent Multiple Scattering method has been used to determine the coupling between all pairs of metal atoms in the supercell. Here we present the result of this calculation, which shows that metal cluster distribution does affect the calculated transition temperatures of the material.

IC/PP1960/113: **Cycle-to-cycle control of simulated moving bed processes.**

Presenter: Cristian Grossmann (ETH Zürich, Switzerland)
Co-author: Mohammad Amanullah (ETH Zürich, Switzerland)
Co-author: Marco Mazzotti (ETH Zürich, Switzerland)
Co-author: Massimo Morbidelli (ETH Zürich, Switzerland)
Co-author: Manfred Morari (ETH Zürich, Switzerland)

Simulated moving bed (SMB) is a continuous chromatographic separation technique that offers high productivity and low solvent consumption. SMB has gained importance in the pharmaceutical and fine chemical industry to perform difficult separation tasks, like purification of chiral molecules for single enantiomer drug development. However, an automatic control algorithm for SMB units that guarantees an optimal, robust operation is still an open and challenging problem because of the complex dynamics involved in this process; e.g., its cyclic and hybrid nature of inlet/outlet port switching, with nonlinearities and delays.

We have developed a control scheme that integrates both, the optimization and control of the SMB unit. The control problem is formulated as a constrained dynamic optimization problem within the repetitive model predictive control framework. The controller predicts and optimizes the future inputs over a given horizon of time by making use of a linear time-invariant cycle to cycle SMB model derived from the system of PDEs describing the process. This scheme is implemented according to a receding horizon strategy; i.e., a new optimization problem based on the latest estimate of the plant state is solved as new measurements are available. The state estimate is computed using a linear Kalman filter. This approach provides the flexibility to apply the controller to a wide range of separation tasks, regardless of the type of isotherm characterizing the mixture or the operation mode of the SMB unit, i.e. synchronized or asynchronized switching of the ports.

This work presents the mathematical development of the cycle to cycle controller. Its performance is illustrated through simulations and experiments that show how the controller fulfills the product and process specifications while operating the SMB unit optimally, regardless of the uncertainties in the parameters of the system or the disturbances.

12: Bio-Mathematics, Minisymposia

IC/MP243/012: Computational methods and investigations in cardiac modeling.

Organiser: Jacques Beaumont (Binghamton University, USA)

Being the number one killer in most industrialized countries, death due to cardiac arrhythmias constitutes a health problem of considerable extent. Over an average life time the human heart beats about 3×10^9 times. Beat after beat the heart performs its function despite numerous disturbances. However, although robust to most perturbations, the heart remains fragile to specific ones. For example several mutations in genes encoding cardiac proteins produce relatively small changes in membrane current kinetics still such minor changes can generate fatal arrhythmias. Also puzzling is the individual variability. For a number of years life science scientists have been puzzled by the fact that the first manifestation of an electrical disturbance occurring in a context of coronary artery disease is fatal to some individuals but not to others. Understanding the source of such sensitivity as well as the individual variability is very much at the basis of developing better interventions. Over the years it has become clear that: the detailed cell membrane current kinetics, the large scale of the system, its complex anisotropy, and convoluted geometry play equally important roles in the setting of arrhythmias. Due to the multifactorial/multiscale nature of the mechanisms of arrhythmias it is not possible to progress on this problem solely on the basis of experimentation. Along this line of thinking, this symposium presents mathematical and computational methods that allow to cope with the multifactorial/multiscale nature of this problem. Furthermore the speakers present several investigations where an elaborate methodology is applied to elucidate the mechanisms of arrhythmias. Overall the symposium material constitutes mathematical approaches allowing to capitalize on the genome, and various cardiac imaging modalities in our venture to develop better therapeutic interventions.

Inversion of Markov processes in bioelectricity: implications for cardiac modelling. **Jacques Beaumont** (Binghamton University, USA), Nikolauss Szeverenyi (Upstate Medical University, USA), David Feiglin (Upstate Medical University, USA) IC/MT275/012

We address the problem associated with the estimation of the voltage dependent transition rates $\vec{\alpha}(u)$ of Markov models utilized in the description of channel gating. We cast this problem in a computational framework aiming at elucidating the mechanisms of life threatening arrhythmias in the entire heart.

Simulation of electric conduction is carried out with a pair of reaction diffusion equations (Bidomain) coupled through their source term with ordinary differential equations (ODEs). These ODEs are mainly composed of Markov models of channel gating. This formalism being empirical, $\vec{\alpha}(u)$ are estimated from experimental data collected in isolated cells (voltage clamp data). The experimental data being the solution of the Markov model in simple conditions, this is clearly an inverse problem. Assuming $\vec{\alpha}(u)$ parameterized with a linear combination of cubic B-splines, we present an inversion method permitting to obtain the coefficients of the expansion through recurrent matrix operations. Considering voltage clamp data sets generated with experimental protocols commonly employed in electrophysiology, our inversion method shows that the Markov gating model is not sufficiently constrained. However the number of inversion solutions is finite, and can be determined systematically.

We assess the implications of the non-uniqueness of the inverse solution of Markov gating models in the simulation of scroll waves anchoring, which is an important mechanism of arrhythmias. Considering multiple inverse solutions lead to a wide range of predictions regarding the interval of time a scroll wave remains anchored. Based on our inversion method we discuss ways to generate voltage clamp data sets that could fully constrain Markov models of channel gating. The availability of such data could dramatically improve the accuracy of the predictions of large scale simulations of electric conduction in the heart.

Simulations of normal and reentry dynamics with mono-domain and bi-domain cardiac models. **Luca Pavarino** (Università degli Studi di Milano, Italy), Piero Colli Franzone (Università degli Studi di Pavia, Italy), Bruno Taccardi (University of Utah, USA), Simone Scacchi (Università degli Studi di Pavia, Italy) IC/MT301/012

We present the results of large-scale parallel simulations obtained integrating two advanced multiscale models in electrocardiology, the anisotropic Bidomain model of cardiac tissue, a degenerate system of two parabolic reaction-diffusion equations, and the Luo-Rudy ionic model, a system of several ordinary differential equations. The simpler anisotropic Monodomain model is also considered. The resulting coupled model includes orthotropic anisotropy, transmural fiber rotation and homogeneous or heterogeneous intrinsic membrane properties, due either to the presence of midwall cells (M-cells) with different APDs or to the presence of subendocardial ischemic regions. Various dynamical features of the model are investigated, for both normal and reentry dynamics, yielding detailed results on recovery and APD dispersions.

Orthotropic and heterogeneous models of the cardiac bioelectric activity. **Piero Colli Franzone** (Università degli Studi di Pavia, Italy), Luca Pavarino (Università degli Studi di Milano, Italy), Simone Scacchi (Università degli Studi di Pavia, Italy), Bruno Taccardi (University of Utah, USA) IC/MT313/012

We consider a mathematical model on a periodic cellular assembling of the tissue and we derive a macroscopic model called *bidomain* using tools of Γ-convergence theory. The *bidomain* model consists in a degenerate reaction-diffusion system coupled with an ordinary differential system and their simulation in 3-dimensional geometry with twisted anisotropy exhibits considerable numerical difficulties and complexity in order to cover the entire range of cardiac electrodynamics behavior. We briefly describe some relaxed approaches: the anisotropic geometric evolution laws capturing the motion of the excitation wavefronts and the anisotropic *monodomain* models. We introduce a splitting of the cardiac current sources which provides a tool for the explanation of the potential patterns and of the multiple waves appearing in the electrograms. We discuss the combined effect of i) the anisotropic electrical conduction, ii) the fiber rotation and iii) heterogeneous intrinsic properties of the cell membrane on the excitation spreading, the potential maps and electrograms elicited by a local stimulus.

Simulating the initiation and control of re-entrant arrhythmias in human virtual ventricles. **Arun Holden** (University of Leeds, UK) IC/MT3297/012

An electrophysiological virtual cardiac tissue is an anatomically (size, geometry, fibre orientation and sheet structure) and spatially heterogeneous, biophysically (kinetics of membrane ion channels, pumps and exchangers, and intracellular ion binding and sequestration) detailed computational model. It is in the form of a reaction diffusion partial differential equation. The reaction term is stiff, high order and exhibits threshold behaviours, and is obtained from voltage clamp experiments on single cells and ion channels in isolated membrane patches. The diffusion term is a tensor describing anisotropy and orthotropy in propagation that results from the fibre orientation and sheet structure of the ventricular wall, that is obtained from quantitative histology or diffusion tensor magnetic resonance imaging. We have constructed such a virtual tissue for the electrophysiology of the human ventricles, and use it to evaluate, and dissect in space and time, candidate mechanisms for the initiation and control of arrhythmias, ventricular tachycardias and fibrillation. In both of these life threatening arrhythmias re-entrant propagation occurs in which the same excitation wavefront repeatedly invades the same piece of tissue. In simple excitable media models re-entry is caricatured by spiral waves in 2D, and scroll waves in 3D. Using high performance computing we simulate the initiation, evolution and termination of ventricular fibrillation in the normal and modified (inherited channelopathies, effects of antiarrhythmics) ventricular wall.

Work done in collaboration with Drs. Oleg Aslanidi (Manchester), Alan Benson (Leeds) and Richard Clayton (Sheffield).

IC/MP28/010: Stochastic aspects of bifurcation and multi-stability in gene regulation.

Organiser: Wilhelm Huisinga (National University of Ireland, Maynooth)
Co-organiser: Michael Mackey (McGill University, Canada)

Modelling and simulation has become the focus of the pharmaceutical industry, driven by the emerging consensus that *in silico* predictions, combined with *in vitro* data, have the potential to significantly increase insight into physiological processes and their pharmacological modification. Studying cellular processes involved in a drug's effect at the target site are of particular interest due to large attrition rates in the clinical trail phases of drug certification. The effect of a drug depends on its potency to qualitatively alter the cellular system or pathways involved. Identification, analysis and understanding of the dynamic switching behavior and bifurcation pattern of cellular processes are therefore of major interest.

This minisymposium focusses on mathematical techniques to identify, analyse and understand multistability and qualitative switching of cellular processes. It aims to bring together mathematical approaches based on deterministic as well as stochastic models, focussing both on the modelling approaches and the techniques suitable to analyse those models.

Stochasticity and designs of genetic networks. **Peter Swain** (McGill University, Canada) IC/MT2600/010

Biochemical reactions are significantly stochastic. Stochasticity has been quantified by using fluorescent reporters in both bacteria and simple eukaryotes. Given its magnitude in vivo, it is at first puzzling how cells reliably process information: how can a signalling network, whose components have concentrations that fluctuate in an unpredictable manner, generate predictable cellular behaviour? I will propose two network designs that aid information processing and flow in biochemical networks. The first, translational feedback, efficiently controls intrinsic noise in network components. The second is a genetic network that enables a cell to classify the state of its environment from intracellular concentrations despite extrinsic noise. Finally, I will highlight an experimental technique that harnesses intrinsic noise to quantify numbers of fluorescently tagged proteins.

Origin of bistability in the lac *operon.* **Moisés Santillán** (Unidad Monterrey, Mexico), Michael Mackey (McGill University, Canada), Eduardo Zeron (Unidad Monterrey, Mexico) IC/MT1021/010

Multistability is an emergent dynamic property that has been invoked to explain multiple co-existing biological states. In this, work we investigate the origin of bistability in the *lac* operon. To do this, we develop a mathematical model for the regulatory pathway in this system and compare the model predictions with the experimental results of Ozbudak *et al.* (*Nature* 427, 737-740, 2004), in which a non-metabolizable inducer was employed. We investigate the effect of lactose metabolism using this model, and show that it greatly modifies the bistable region in the external lactose (Le) *vs.* external glucose (Ge) parameter space. The model also predicts that lactose metabolism can cause bistability to disappear for very low Ge. We have also carried out stochastic numerical simulations of the model, for several values of Ge and Le, to analyze the effects of intrinsic noise due to small numbers of regulatory molecules. Our results indicate that bistability is an efficient way to guarantee that *E. coli* consumes glucose and lactose in the most efficient possible way. Namely, the *lac* operon is induced only when there is almost no glucose in the growing medium, but if Le is high, the operon induction level increases abruptly when the bacterial culture is virtually depleted of glucose. We demonstrate that this behavior could not be obtained without bistability if the stability of the induced and uninduced states is to be preserved. Finally, possibility of using the present methods and results to study the emergence of multistability in biological systems other than the *lac* operon.

Near-critical fluctuations in pathways with coupled flux. **Johan Elf** (Harvard University, USA) IC/MT1486/010

I will discuss the near-critical properties of unsaturated multi-substrate reactions [1,2]. In essence, one substrate pool can decrease while another increases, such that the overall flux remains unchanged. This results in high sensitivity in substrate concentrations to flow imbalances, but it also induces large zero order fluctuations in several dimensions. The near-critical properties of coupled flow processes are predicted to have important consequences for the flow of different amino acids into proteins synthesis [3]. In particular I will discuss the implication for transcriptional control of amino acid biosynthetic operons.

If there is time I will also discuss noise induced domain separation in spatially extended bi-stabile systems [4].

1. Elf J., Paulsson J., Berg O. & Ehrenberg M.(2003) Near-critical phenomena in intracellular metabolite pools *Biophysical Journal* **84** 154-170

2. Elf, J and Ehrenberg, M (2003) Fast evaluation of fluctuations in biochemical networks with the linear noise approximation *Genome Research* **13** 2475-2484

3. Elf, J and Ehrenberg, M (2005) Near-critical behavior of aminoacyl-tRNA pools in E. coli at rate limiting supply of amino acids*Biophys. J* **88** 132-46

4. Elf, J and Ehrenberg, M (2004) Spontaneous separation of bi-stable biochemical systems into spatial domains of opposite phases. *IEE Systems Biology* **1** 230-235 http://mesord.sourceforge.net/references/ElfSysBio.pdf

Discrete methods for the qualitative modeling of regulation networks. **Ron Pinter** (Technion – Israel Institute of Technology) IC/MT2999/010

Modeling and analysis of genetic regulatory networks is essential both for better understanding their behavior as well as for elucidating and refining open issues. To this end, a model needs to effectively reflect important qualitative characteristics such as transient expression, robustness, and sensitivity to initial conditions. We describe discrete computational models that allow for such qualitative analyses of regulatory pathways in an effective manner without the need for detailed quantitative data.

Our primary computational tools are discrete transition systems. A system's next state is determined by a set of simple transition rules that reflect both the interactions that govern regulation as well as the conjunctive conditions that enable them. The synchronous application of the transition rules — first to an initial vector and then repeatedly onwards — constitutes a simulation of the system's behavior. We used a variety of techniques, including Karnaugh-like maps, to analyze the functional relation between the initial states and their type of behavior.

We have applied our methods to analyze the transience and robustness of several representative developmental pathways, *e.g.* the transcription of meiosis-specific genes in budding yeast; our simulations suggested a new mode for the negative feedback regulation in this system, which was verified experimentally. In general, our methods provide insights into how to distinguish among and reason about alternative hypotheses concerning the function and structure of regulatory networks.

IC/MP210/010: Emerging challenges in mathematical biology.

Organiser: David Kinderlehrer (Carnegie Mellon University, USA)
Co-organiser: Emmanuele DiBenedetto (Vanderbilt University, USA)
Co-organiser: Angela Stevens (Universität Heidelberg, Germany)

The synergy between the Life Sciences and mathematics is growing rapidly. Mathematics and Biomedical Sciences will reach soon a common ground and language as deep and fruitful as that present between Mathematics and Physics, Chemistry, Engineering and Material Sciences.

Further progress in understanding basic functional mechanisms ină biology and medicine, and for models to become more predictive, requires a variety of new mathematical methods, and, mostly, a change of investigative mentality. The goal is generate solid and robust models, which, as for Physics, Chemistry and other disciplines, become cornerstones for future developments.

With this in mind, the mini symposium on mathematical biology asks of mathematicians andă experimentalists to present contributions, blending experimental and mathematical challenges in the life-sciences.

Mechanics of biological materials making tendons and ligaments. **Antonio Fasano** (Università di Firenze, Italy) IC/MT1184/010

The material making ligaments and tendons is characterized by a threshold for extensibility, which makes its response to traction nonlinear. Such a behaviour can be described, in the one-dimensional case, by a nonlinear relationship between stress and strain with the stress going to infinity when the strain approaches the threshold. An extrapolation of such a law is considered in which the material is simply linear elastic below the threshold and becomes inextensible at the maximum admissible strain. In this case the transition is also marked by a stress threshold. The corresponding constitutive law has an implicit form. A specific model problem is studied for a layer in which one boundary is kept fixedd, while the other is subject to a shear stress exceeding the threshold value. Two questions are addressed: (i) The mathematical formulation of the corresponding free boundary problem and the existence of solutions, (ii) Whether or not the problem with the implicit constitutive law can be recovered as a limit from the explicit nonlinear elastic formulation. Not surprisingly the mathematical problem takes the form of a free boundary problem for the wave equation, but the conditions at the moving interface can be considerably complicated and have different aspects for subsonic and for supersonic interfaces. Existence and uniqueness are proved for the subsonic case, which however turns out to be of moderate physical interest. The supersonic case is closer to physics, but so complicated that it is left basically open, with the exception of some typical problems, which are solved explicitly. The comparison between the implicit and the explicit model goes through energy considerations. The implicit model can be dissipative, while the explicit model is not (the dissipation rate can be calculated). So the former cannot be the limit of the latter.

Modeling signal transduction through thrombin receptors in endothelial cells. **Heidi Hamm** (Vanderbilt University, USA) IC/MT3180/010

Stimulation of many G protein coupled receptors (GPCR) results in the activation of multiple classes of G proteins. How these individual pathways form interconnected networks modulating each other in a spatio-temporal manner and ultimately integrate to form a single combined response has been largely overlooked by both the biological and mathematical communities. We have developed techniques in our laboratory which allow us to specifically investigate the biochemistry of individual G protein systems induced by promiscuous GPCR. We are connecting these experimental approaches with mathematical modeling of the spatio-temporal aspects of signaling through the thrombin receptor which governs permeability in the endothelium. On endothelial cells, thrombinŠs effects are mediated mainly through activation of PAR-1 by cleaving the amino terminal domain of the receptor, exposing a new terminus. Three classes of G proteins, Gai, Gaq, and Ga12/13, have been shown to by activated by PAR-1. Importantly, each class of G proteins have been shown to be involved in thrombin-induced permeability. Our modeling efforts have shown that this receptor takes on different affinity for the three G proteins based on how it is activated. Thrombin receptor agonist peptides activate PAR-1 in such a way as to enhance $G\alpha q$ signaling pathways, increasing calcium mobilization, and/or decrease $G\alpha 12/13$ signaling pathways leading to endothelial barrier dysfunction.

Variability of the single-photon response in photo-transduction. **Emmanuele DiBenedetto** (Vanderbilt University, USA), Daniele Andreucci (Università degli Studi di Roma "La Sapienza", Italy), Paolo Bisegna (Università degli Studi di Roma Tor Vergata, Italy), Giovanni Caruso (Università degli Studi di Roma Tor Vergata, Italy), Heidi Hamm (Vanderbilt University, USA), Lixin Shen (Vanderbilt University, USA) IC/MT1763/010

The rod outer segment (ROS) in vertebrates consists of a cylinder including a stack of thin discs carrying photoreceptors. The second messengers Calcium and cGMP diffuse in the cytosol, which is the layered domain formed by the ROS from which the discs are ideally removed.

Upon activation the Rhodopsin photoreceptors starts a cascade (receptor-transducer-effector) and undergoes a number of phosphorylation events random in duration, prior quenching at a random shutoff time. The final output is the photocurrent generated by closing of the cGMP-gated channels.

Because of the presence of several random events in the cascade, and in analogy with similar physical processes exhibiting random shutoff times, such as radioactive decay, one might expect that he final output is highly variable (large CV=coefficient of variability).

It is however observed that the CV of the photocurrent at peak time is relatively low.

We explore some reasons for such a low variability, by separating the random effects of the Rhodopsin shutoff events, from the diffusing/stabilizing effects of the second messengers in the cytoplasm

Equation vs. chip: integrative and iterative studies of cell signaling. **Andre Levchenko** (Johns Hopkins University, USA) IC/MT1204/010

Living cells have evolved complex and sophisticated means of detecting and responding to changes in their microenvironment. Loss of the ability to correctly detect and interpret these changes might result in severe disorders, including cancer. Our lab has been engaged in the analysis of cell signaling and cell-cell communication using novel mathematical, computational and experimental tools, including performing experiments with live cells in micro- and nano- fluidic chips. In this talk I will discuss the the recent progress in our analysis of how signaling pathways are organized and how the underlying chemistry supports efficient and robust information transfer.

IC/MP210/010: Emerging challenges in mathematical biology. #2

Organiser: David Kinderlehrer (Carnegie Mellon University, USA)
Co-organiser: Emmanuele DiBenedetto (Vanderbilt University, USA)
Co-organiser: Angela Stevens (Universität Heidelberg, Germany)

(For abstract, see session #1 above.)

Aspects of modeling transport in small systems with a look at motor proteins. **David Kinderlehrer** (Carnegie Mellon University, USA), Michel Chipot (Universität Zürich, Switzerland), Stuart Hastings (University of Pittsburgh, USA), Michał Kowalczyk (Universidad de Chile), Bryce McLeod (University of Pittsburgh, USA) IC/MT1233/010

Motion in small live systems has many challenges. Prominent environmental conditions are high viscosity and warmth. It is difficult to move and maintaining a course is compromised by immersion in a highly fluctuating bath. We discuss some possibilities for motor proteins, which transduce chemical energy into directed mechanical energy. Such nanoscale motors, like conventional kinesin, have a role in intracellular transport, separating the mitotic spindle, and many other cellular functions. Our approach is to formulate a dissipation principle connected to the Monge-Kantorovich mass transfer problem. We show how this leads to a system of evolution equations. We then discuss how various elements of the system must be related in order that transport actually occur.

Multi-scale analysis of systems modelling reactive flow, diffusion and transport through biological membranes and tissue. **Willi Jaeger** (Universität Heidelberg, Germany), Maria Neuss-Radu (Universität Heidelberg, Germany), Andro Mikelic (Université Claude Bernard Lyon I, France) IC/MT2313/010

Modelling flow, transport and reactions of substances in membranes and tissues and their interactions with mechanics of the solid structures on a cellular level lead to a coupled system of nonlinear partial differential equations in complex geometric structures. Taking into account biological information from experiments, characteristic scales are identified. The arising non-standard model system is solved and estimates of the solutions are derived, controlling their dependence on the scale parameter. Using techniques of asymptotic analysis, we investigate the limit to a macroscopic model system under the assumption of periodic structures. By coupling information on the processes in the micro-scale with macroscopic properties we provide theoretical answers to questions posed by physiologists studying experimentally the transport through tissues and cell layers. This lecture is based on joint work with M. Neuss-Radu (Heidelberg) and A. Mikelic (Lyon).

A mathematical approach to biological invasive processes. **Gabriela Litcanu** (University Witten/Herdecke, Germany) IC/MT2308/010

The cell proliferation process is normally closely controlled by several feedback biological processes. Despite of this fact, sometimes the cell populations break away from their primary status through mutations that allow them to spread into surrounding medium. This invasion process involves a number of changes in cells behaviour, in particular changes in motility, adhesion and production of enzymes that will manipulate their local environment. An example is tumour invasion, that enables the cancer cells to break down the surrounding tissue and to move into a blood vessel and be transported through the body. This is a very complex process and several authors, during the last decades, have proposed mathematical models for it.

In this talk we shall discuss some aspects related to mathematical models for the cell invasion processes. Among the aspects we intend to focus on, we mention existence results concerning the solutions of the equations involved and asymptotic behaviour of the solutions. We also intend to present numerical results and a comparison with experimental data will be taken into account.

Mathematical modeling of alignment and aggregation in cell biology. **Angela Stevens** (Universität Heidelberg, Germany), Kyungkeun Kang (Sungkyunkwan University, South Korea, Sud-Korea), Benoit Perthame (École Normale Supérieure de Paris, France), Ivano Primi (Max-Planck-Institut Leipzig, Germany), Juan Velazquez (Universidad Complutense de Madrid, Spain) IC/MT1957/010

Self-organization of cells and filaments is an important process in developing and living tissues. Long-range and short-range signaling as well as mechanical interactions play a role here. A question of major interest is, how the dynamics of pattern formation are influenced by the specific type of cellular interaction.

In this talk we focus on structure formation due to cell motion and alignment. Models of integro-differential-equations will be analyzed with respect to their qualitative behavior, in order to undestand the interplay between structure and function in these interacting cell systems.

IC/MP227/015: The impact of biology on mathematical modelling.

Organiser: Robert Anderssen (CSIRO, Australia)
Co-organiser: Frank de Hoog (CSIRO, Australia)

The role played by mathematics in solving challenging real-world problems is clearly understood. One can find many examples in industrial mathematics. Impact occurs when the matter under investigation leads to a question which can only be answered after further development of new mathematical results.

This process of letting the application dictate how the underlying mathematical models should be formulated, so familiar in industrial mathematical contexts, will play an equally important role in the intefacing of biology with mathematics. Success will depend heavily on collaboration between biologists and mathematicians. The talks in this Minisymposium will explore such matters by first identifying an important biological problem, explaining how mathematics is involved, discuss the essence of this mathematics and finally identify key mathematical questions that need to be resolved in order to advance current understanding.

Modelling the viscoelasticity of cell-shape changes. **Roger Hosking** (Universiti Brunei Darussalam), Saiful Husain (Universiti Brunei Darussalam) IC/MT411/015

Biological processes often involve changes in shape, which may well raise rheological issues. For example, cell deformation occurs in response to forces from the external environment or from within the cell. In tests of cell rheology, an external constraint is usually superimposed on an already mechanically active cell, so the measurements may reflect both active and passive viscoelastic deformation. Experiments provide information on cell deformation under stress, such that a constitutive model for the cell structure may emerge. There are deformation phases with various time scales, which are open to interpretation. A simple Kelvin viscoelastic model has been suggested, but there are other viewpoints.

Inverse bifurcation analysis for gene networks: application to cell cycle and circadian rhythm models. **James Lu** (RICAM Linz, Austria) IC/MT230/015

The use of mathematical models provides a way to understand the complex interaction of genes regulating the metabolism of living cells. Given ODE models for gene regulatory systems, one may ask the question: how does the qualitative behavior of the regulatory system arise, from parameter choice, network topology, or both? To address such questions we propose the methodology of inverse bifurcation analysis, based on mapping the space of bifurcation diagrams back to the space of parameters and networks.

We show that sparsity-promoting regularization strategy, in combination with numerical bifurcation analysis, can be used to identify small sets of "influential" submodules and parameters within a given network. In addition, hierarchical strategies can be used to generate parameter solutions of increasing non-zero components. We demonstrate the proposed method in addressing some biological questions arising from models of cell cycle and circadian rhythm.

An inverse problems approach to the identification of the chemotaxis response function. **Philipp Kuegler** (RICAM Linz, Austria) IC/MT367/015

Chemotaxis is the directed motion of cells in response to the gradient of a chemical attractant. Modeling of the cell flux due to chemotaxis typically involves a chemotaxis response function depending on the attractant concentration. However, different ideas about its functional form can be found in the literature. In this talk we consider the determination of the functional form of the chemotaxis response as a nonlinear inverse problem. We discuss Tikhonov regularization for its solution and present numerical results both for simulated and experimental cell density data.

Approximate solutions of differential equations in biosensors models. **Frank de Hoog** (CSIRO, Australia) IC/MT1603/015

The response of biosensors can be modeled using an electrical network with a number of switches, where their density can be modeled as the solution of a system of differential equations. However, while there is no difficulty in obtaining numerical solutions to these differential equations, it is often difficult to interpret the results of these simulations. This talk will focus on obtaining an improved understanding of the maximal rate of response. Specifically, for typical biosensor parameters:

- A number of simplifications to the underlying system of ordinary differential equations are derived
- A simple algebraic expression for the maximal rate of response when the analyte concentration is high is derived
- A simple algebraic expression for the maximal rate of response when the analyte concentration is low is derived
- A simple algebraic expression for the maximal rate of response, which is valid in an asymptotic sense for the complete range of analyte concentrations of interest is derived

This is an illustration of how an important industrial biology problem has impacted on the mathematics that models the essence of the process under investigation.

IC/MP227/015: The impact of biology on mathematical modelling. #2

Organiser: Robert Anderssen (CSIRO, Australia)
Co-organiser: Frank de Hoog (CSIRO, Australia)

(For abstract, see session #1 above.)

The EM algorithm for PET: a regularization approach. **Elena Resmerita** (RICAM Linz, Austria), Robert Anderssen (CSIRO, Australia) IC/MT2294/015

Positron emission tomography (PET) is a powerful technique for assessing physiological parameters such as blood flow and metabolism, based on measuring concentration of radiotracers. The EM algorithm for image reconstruction in PET has a simple form, being frequently used in practice. In this presentation, we consider the algorithm in an infinite dimensional setting and approach it via regularization, which allows us to investigate its convergence and to deal with its instability.

Modelling pattern formation in plants. **Robert Anderssen** (CSIRO, Australia) IC/MT1397/015

The history of studying pattern formation in biology can be traced back to Fibonacci and phyllotaxis. Though much has been written on this subject, the mechanism of the genetic control of the geometry of pattern formation in plants, such as the spacing of trichomes on Arabidopsis leaves, remains an open question. From a macroscopic perspective, Turing's seminal 1952 paper on morphogenesis represents the starting point for the various partial differential equation, reactor-diffusion, models that have been proposed for pattern formation in biology. Though such models can be adapted to simulate observed biological patterns, the activator-inhibitor mechanisms, on which they are based, have yet to be observed biologically. A new mathematical approach is required which responds to, and explains the role of, the dynamics of the plethora of genes involved in biological development in terms of the results from mutant experiments. A model for the control of the spacing of the trichomes on Arabidopsis leaves will be presented.

Stochastic delay modelling and simulation of cellular signalling and genetic regulation. **André Leier** (University of Queensland, Australia), Kevin Burrage (University of Queensland, Australia), Manuel Barrio (Universidad de Valladolid, Spain) IC/MT4139/015

Time delays associated with slow biochemical processes such as transcription, translation, nuclear and cytoplasmic translocations are known to affect the dynamics of genetic regulation. Temporal models of cellular signalling and genetic regulation have to take these delays into account in order to capture the dynamics more accurately and to allow for more reliable predictions.

Recently, transcriptional and translational delays have been studied and modelled for autoregulated oscillating genes using delay differential equations (DDEs). However, in this modelling regime we assume large numbers of molecules for each species which enables us to talk about concentrations instead of numbers of molecules. The dynamics is deterministic and is not suitable for modelling stochastic effects that are due to small numbers of molecules and the uncertainty of knowing when a reaction occurs and which reaction it is.

In this talk, we discuss stochastic delay modelling and simulation suitable to capture both stochasticity and delay in temporal models of cellular signalling and genetic regulation. Here, we focus on delayed feedback-loops in the genetic regulation of hes1 and her1/her7, genes that are known to play key roles as molecular clocks during somite segmentation in Mouse and Zebrafish.

The use of hydrodynamics to help understand biological hazards in estuaries . **Stephen Roberts** (Australian National University) IC/MT4154/015

We will present our efforts to use hydrodynamic modelling of esturies to better understand the development of biological hazards (nutient overload, leading to toxic blooms, increased pathogen concentrations). We would like to gain an understanding of the correlation of typical hydrodynamic measures such as resident times to the development of biological hazards. A discussion of coupled hydrodynamic, pathogen and nutient models will be presented.

IC/MP222/015: Dynamics of gene regulation.

Organiser: Tomáš Gedeon (Montana State University, USA)
Co-organiser: Konstantin Mischaikow (Rutgers University, USA)

Understanding function and control of gene regulation is at the center of current efforts in molecular and systems biology. The importance of the dynamics of this regulation is evident by the fact that not only do cells and organisms display internal cycles and rhythms, but also live in and therefore must respond to constantly changing environments.

The speakers in this Minisymposium will describe different approaches to modeling the dynamics of associated with gene regulation at a variety of levels and in a variety of organisms.

Mathematical modeling of gene regulation. **Michael Mackey** (McGill University, Canada) IC/MT1607/015

This talk will focus on mathematical models of inducible and repressible operons, and the variety of dynamic behaviours that these gene regulatory networks may display. Concrete examples will be drawn from the lac operon, the tryp operon, the lysis-lysogeny switch in phage lambda, and the developmental oscillations in Hes1 expression.

Dynamics of a simple regulatory switch. **Tomáš Gedeon** (Montana State University, USA), Konstantin Mischaikow (Rutgers University, USA) IC/MT1573/015

We consider the dynamics of a model toggle switch abstracted from the genetic interactions operative in a fungal stress response circuit. The switch transduces an external signal and propagates it forward by mediating the transport between compartments of two interacting gene products. The transport between compartments is assumed to be related to the degree of association between the interacting proteins, a fact for which there exists a wealth of biological evidence. The ubiquity and modularity of this cellular control mechanism warrants a detailed study of the dynamics entailed by various modeling assumptions. Specifically, we consider a general gate model in which both of the associating proteins are freely transportable between compartments. A more restrictive, but biologically supported model, is considered in which only one of the two proteins undergoes transport. Under the strong assumption that the disassociation of the interacting proteins is unidirectional we show that the qualitative dynamics of the two models are similar; that is they both converge to unique periodic orbits. From a biophysical perspective the assumption of unidirectional dissociation is unrealistic. We show that the same result holds for the more restrictive model when one weakens the assumption of unidirectional binding or disassociation. We speculate that this is not true for the more general model. This difference in dynamics may have important biological implications and certainly points to promising avenues of research.

Gene regulation during cell-fate decisions in bacillus subtilis. **Dagmar Iber** (Imperial College London, UK) IC/MT2626/015

Sporulation in *Bacillus subtilis* serves as a paradigm for the development of two different cell types from a single cell. The key event is the selective activation of the transcription factor sigmaF in the smaller prespore but not in the larger mother cell. We have recently developed a comprehensive quantitative model which showed that the difference in volume between the two cell types is sufficient to function as the primary trigger for determining cell fate. The model predicted that this switch depended on the allosteric behaviour of a key protein kinase and on a low rate of dephosphorylation by the corresponding phosphatase; both effects were confirmed experimentally. The same network architecture is employed in the regulation of

the general stress response although the trigger is necessarily very different. With the help of the quantitative model we can explain how such small regulatory network not only achieves an exceptionally high sensitive to input but is also readily adjustable to respond to different types of triggers.

Experimental and modeling approaches for the analysis of the spindle assembly checkpoint. **Andrea Ciliberto** (Istituto FIRC di Oncologia Molecolare, Italy) IC/MT3750/015

The spindle assembly checkpoint (SAC) ensures that the metaphase-to-anaphase transition occurs only when all chromosomes undergo bipolar attachment with the microtubles emanating from the spindle pole bodies. By doing so, the SAC prevents the formation of cells with an uneven number of chromosomes (aneuploidy), a phenomenon known to play an important role in cancer development. Interestingly, the SAC is activated even by a single unattached kinetochore, a fact that suggests the presence of a catalytic step that amplifies the signal originated from unattached kinetochores. Several pieces of this mechanism have been identified in recent year, but still a proper molecular understanding of the process is awaiting. With a combination of experiments in vitro and mathematical modeling, we propose a model for the SAC based on autocatalysis. The molecular network we describe involves a subset of the molecules known to be involved in the SAC; nevertheless it is able to describe in qualitative and quantitative detail the main properties of the SAC.

Work done in collaboration with Andrea Musacchio, Romilde Manzoni, Marco Simonetta, Marina Mapelli.

IC/MP222/015: Dynamics of gene regulation. #2

Organiser: Tomáš Gedeon (Montana State University, USA)
Co-organiser: Konstantin Mischaikow (Rutgers University, USA)

(For abstract, see session #1 above.)

Monotone dynamics in gene regulation. **Hal Smith** (Arizona State University, USA) IC/MT3775/015

Monotone dynamical systems theory has played a prominent role in the analysis of simple models of gene regulatory networks. We will survey this work and presnt new results.

On a system reduction for positive feedback networks. **German Enciso** (Ohio State University, USA), Eduardo Sontag (Rutgers University, USA) IC/MT2773/015

A control-theoretic approach has been introduced by Sontag and Angeli to study positive feedback (monotone) networks, by considering an associated input-output system and studying its steady input response function k(x). In this talk it is illustrated that a one-dimensional reduction of the original system is sometimes possible even if k(x) is not single-valued. An application is given to the case of hysteresis on the input variable.

Molecular seismology: an inverse problem in nano-biology. **Peter Hinow** (Vanderbilt University, USA), Erik Boczko (Vanderbilt University, USA) IC/MT3776/015

An obstruction to progress in modeling the dynamics of regulatory networks has been the lack of quantitative time series data for the many molecular processes that are operative during gene expression. Virtually nothing is understood about the dynamics of transcription factor competition at and around individual promoter sequences and the pervasive modeling assumption has been to invoke quasi-equilibrium based on separation of timescales. In considering the modeling problems posed by the members of the GATA family of transcription factors we were led to develop a single molecule assay strategy that can in principle measure the dynamics of association between an arbitrary ligand such as a protein and an elastic fiber like DNA. The assay is based on the following simple observation: the density profile of an elastic fiber like DNA will change in space and time as ligands associate with it. This observation affords a new direction in single molecule studies provided that density profiles can be measured in space and time. In fact, this is precisely the objective of seismology, where the mathematics of inverse problems have been employed with success. We argue that inverse problems in elastic media can be directly applied to biophysical problems of fiber-ligand association, and demonstrate that robust algorithms exist to perform density reconstruction in the condensed phase.

Why does the positive regulation in bacteriophage λ affect isomerization of the RNAP–DNA complex?. **Kate Patterson** (Montana State University, USA) IC/MT4864/015

Bacteriophage λ is the best studied example of a gene regulation switch. The phage-infected cell can follow the lytic pathway which leads to production of new phages and lysis of the cell. Alternatively, the infected cell can follow the lysogenic pathway, in which the virus establishes stable association with the host. In the last 20 years a number of experiments elucidated gene regulation mechanisms that are behind the choice of alternative states and their maintenance.

The transcription initiation involves two distinct steps; first RNA polymerase binds the promoter to form an unstable, closed complex (this reaction is described by an equilibrium constant K_B); second the closed complex isomerizes to an active, stable open complex (the reaction is described by a forward rate constant k_f). The cooperativity between CI protein and RNA polymerase is accomplished by DNA bound CI increasing the forward rate constant k_f about 10-fold without having any significant effect on K_B.

We use a model due to Santillian and Mackey, which is based on Ackers chemical equilibrium description of the promoter binding by the regulatory factors, to show that the stability of the lysogen will be severely compromised if CI had the 10-fold effect on K_B and no effect on k_f.

We also discuss the underlying reasons for this highly nonlinear and counterintuitive effect.

IC/MP266/015: Computational and statistical methods in cell biology.

Organiser: Erkki Somersalo (Teknillinen Korkeakoulu, Finland)

In this minisymposium we discuss numerical and statistical methods applied to problems arising in systems biological models for cell metabolism. The biochemical pathways in different cell types constitute a complex system that depends on a large number of parameters that should be estimated from scarce and imprecise data such as biopsies. The problems are severely ill-posed and underdetermined, and it is of crucial importance to import *a priori* information to reduce the degree of underdeterminacy as well as develop efficient model reduction techniques to make the parameter estimation problem feasible. A combination of numerical and statistical methods is needed to this task. In the minisymposium, recent developments in this area is precented.

Bayesian flux balance analysis. **Knarik Tunyan** (Teknillinen Korkeakoulu, Finland), Jenni Heino (Teknillinen Korkeakoulu, Finland), Daniela Calvetti (Case Western Reserve University, USA), Erkki Somersalo (Teknillinen Korkeakoulu, Finland) IC/MT1218/015

One of the challenging questions in the last decade is to understand the metabolism of the living organisms, i.e., the complex biochemical structure and functions within an organ, as well as relation between different organs. This problem can be formulated as an estimation of the reaction and transport fluxes, when the biochemistry within an organ is known and bound constraints for the fluxes are given. The problem has been addressed previously by a number of authors, and different approaches have been proposed. The steady state condition, when the system under consideration is at rest, can be described by underdetermined system of linear equations with boundary constraints, whereas the dynamics of biochemical reactions and transport processes of metabolism can be represented as a system of ordinary differential equations. Both cases involve a large number of parameters.

The computed solution depends on the input data, which may contaminated by measurement errors and/or fluctuate over a population. Thus, the determination of a unique set of model parameters in both steady state and dynamic cases, based on uncertain data, is usually not possible. Our approach to this problem allows the incorporation of various levels of uncertain information into the model.

The base of our analysis is Bayesian statistical approach and the Markov Chain Monte Carlo techniques. We show that the Bayesian framework can be applied to the flux balance analysis, and the available data can be incorporated into the model by proper construction of the prior densities.

We also address the questions about how the given organ behaves under different conditions, such as physical exercise, diabetic conditions, hypoxia and ischemia.

The obtained solutions are compared with the existing approaches.

Inverse eigenvalue analysis of eukaryotic GATA transcription factor system. **James Lu** (RICAM Linz, Austria), Rainer Machné (Universität Wien, Austria) IC/MT2417/015

Transcription factors can form auto-regulatory feedback cycles by modulating their own expression. By both experimental and theoretical analysis, auto-activating feedback systems have been observed to exhibit bistable behavior. Similar feedback loops, involving both activating and repressing transcription factors, are thought to underly central cellular oscillatory behavior (including the cell division cycle).

In this work, we investigate the possibility for the emergence of new dynamical behaviors through plausible evolutionary transition scenarios for the eukaryotic GATA transcription factor system. This system is known to function as a bistable gene switch and is suspected to be a central regulatory motif in cell-wide oscillatory phenomena. The biologically important questions include: how does the proposed simple evolutionary transition affect bistability? Can oscillations arise from a bistable switch by gene duplications and simple mutations? We propose an inverse method based on sparsity-promoting regularization to computationally investigate these issues.

Dynamic Bayesian sensitivity analysis in myocardial metabolism. **Rachael Hageman** (Case Western Reserve University, USA), Daniela Calvetti (Case Western Reserve University, USA) IC/MT3222/015

The dynamics of biochemical reactions and transport processes in the myocardial metabolism is described by a three-compartment model specified by a large number of parameters. The temporal behavior of some of these reactions and processes during ischemia is not well understood. The available data for the dynamic response of the system during ischemia is scarce and by its own nature statistically distributed. In particular, the distribution of enzyme facilitators $FADH_2$, FAD, NAD+, NADH, ATP and ADP between cytosol and mitochondria are difficult to measure and compartmentalize. We use integrated numerical and statistical techniques to study the sensitivity of the redox and phosphorylation states in both cytosol and mitochondria to the malate-aspartate shuttle and processes including glycolysis, oxidative phosphorylation, lactate production and the transport of chemical species between compartments.

Simulating intercellular calcium and inositol-1,4,5-trisphosphate *signaling in systems of epithelial cells using multiblock grids.* **Petri Fast** (Lawrence Livermore National Laboratory, USA) IC/MT3387/015

We model the biochemical wave dynamics of calcium mediated by inositol 1,4,5-trisphosphate(IP3) in connected epithelial cells. We present a new computational framework that allows for the first time fully three dimensional simulations of the interplay between calcium dynamics, IP3 and calcium buffering species in coupled *in silico* cells represented by structured multiblock grids. Intercellular connections between epithelial cells are modelled using a geometrically realistic computational mesh with a simple continuum description of gap-junctions permeable to IP3. Practical grid generation techniques are discussed for cuboidal epithelial cells consisting of a single layer of three dimensional coupled prismatic domains, each with an arbitrary polygonal top (apical) surface. A novel numerical scheme is presented for modeling diffusion on structured multiblock grids with "gap-junction boundary conditions," where the normal flux across a membrane separating two cells is proportional to a jump in the local concentration. We present results illustrating the range of biological phenomena accessible to these simulation techniques.

IC/MP267/121: Multi-strain diseases: from predictive modeling to vaccine control.

Organiser: Lora Billings (Montclair State University, USA)
Co-organiser: Ira Schwartz (U.S. Naval Research Laboratory)
Co-organiser: Derek Cummings (Johns Hopkins University, USA)

As we become more sophisticated in our resources to fight viral disease, pathogens have shown an exceptional ability to adapt to overcome our attempts to defeat them. From influenza to dengue to pneumoccocus, pathogens have utilized genetic diversity and mutability to escape human's immune defenses. The persistence of influenza depends on its ability to evolve into new strains and subtypes, keeping ahead of natural and vaccine derived immunity. In dengue, antibody-dependent enhancement increases viral replication in the presence of pre-existing immunity, possibly increasing the infectiousness of second infections. This mini-symposium will bring together mathematical researchers, biologists, and epidemiologists to discuss the development of mathematical methods to model the dynamics multi-strain diseases. Using these models, vaccination strategies can be formulated, tested and evaluated in a wide variety of circumstances. Mathematical methods and techniques for analysis and vaccine control will be highlighted along with the models.

The interplay between protective and disease enhancing immunity in the temporal dynamics of dengue. **Derek Cummings** (Johns Hopkins University, USA) IC/MT2704/121

Dengue fever is caused by a mosquito-borne virus of the flavivirus family. The virus causes substantial morbidity and mortality around the globe. Four antigenically distinct serotypes exist. All four circulate in most endemic areas. Sequential infections with multiple serotypes are associated with severe disease -particularly the hemorrhagic form of dengue infections, dengue hemorrhagic fever (DHF) through an immune mediated mechanism. Though immunity is associated with severe disease, it is clear immunity also provides protection from infection under different circumstances. The interplay between protective and disease enhancing immunity is not understood especially at a population level. Four types of immune response are potentially important for dengue; long-term serotype specific immunity, short-term cross-serotype immunity, immune enhancement of secondary infection and dengue-specific, long-term cross-serotype immunity. In this work, I explore the effect of different host/pathogen interactions on population level dynamics of disease incidence using both deterministic and stochastic models. Model outcomes include phase relationships between each of the serotypes and the periodic behavior of different model systems. Simulation results are compared to data from Thailand where all four serotypes of the disease co-circulate.

Why do virulent lineages of bacterial pathogens persist?. **Sunetra Gupta** (University of Oxford, UK) IC/MT2301/121

Populations of pathogenic bacteria commonly contain *lineages* or groups of related organisms, typically defined by non-random associations of alleles at loci which encode housekeeping functions. The presence of these lineages cannot be ascribed to asexual reproduction as many of these pathogens undergo frequent genetic exchange. Rapid clonal expansion can explain the short term domination of a recombining population by a limited number of lineages, but it cannot account for their persistence. Here we propose a theoretical framework which explains both the persistence of lineages in recombining populations and the association of some of these lineages with a propensity to cause disease without invoking a link between mechanisms of transmission and disease.

Desynchronization and spatial effects in multi-strain diseases. **Leah Shaw** (U.S. Naval Research Laboratory), Lora Billings (Montclair State University, USA), Ira Schwartz (U.S. Naval Research Laboratory), Derek Cummings (Johns Hopkins University, USA) IC/MT2655/121

Dengue fever, a multistrain disease, has four distinct coexisting serotypes. The serotypes interact by antibody-dependent enhancement (ADE), in which infection with a single serotype is asymptomatic, but contact with a second serotype leads to serious illness accompanied by greater infectivity. It has been observed from serotype data that outbreaks of the four serotypes occur asynchronously (Nisalak et al., Am. J. Trop. Med. Hyg. 68: 192). We present a compartmental model for multiple serotypes with ADE, and consider autonomous, seasonally driven, and stochastic versions of the model. For sufficiently small ADE, we find that the number of infectives of each serotype synchronizes, with outbreaks occurring in phase. However, when the ADE increases past a threshold, the system becomes chaotic, and infectives of each serotype desynchronize. Certain primary and secondary infective compartments remain synchronized in the chaotic regime, a result which is explained by our analysis and which may be useful for disease monitoring. Spatial effects are included via coupled patch models. We observe desynchronization between spatially distinct regions.

Incorporating realistic genetics in simple models of multi-strain pathogens. **Neil Ferguson** (Imperial College London, UK) IC/MT2431/121

Modelling the transmission dynamics of antigenically variable pathogens poses a key challenge: the exponentially growing dimensionality of the dynamical equations as the number of strains being modelled increases. To avoid this problem, most past deterministic modelling of multi-strain pathogens has made highly simplifying assumptions. Another approach has been to use individually-based microsimulations which explicitly track all members of the host population and their infection history. This has been highly successful at reproducing observed patterns of antigenic evolution of human influenza viruses and giving insight into the immunological mechanisms driving those evolutionary patterns. However, simulation models are far from transparent, so it would be advantageous to be able to bridge the gulf between simple deterministic models and simulations. In pursuit of this goal, we have developed a new set of deterministic multi-strain models with genetic structure in which cross-immunity is determined (in an arbitrary manner) by the degree of genetic overlap between past strains and the new challenge strain. In addition we have incorporated stochastic elements within the model Ü in modelling mutation as the random introduction of new strains, and by modelling extinction as the elimination of a strain when its prevalence drops below 1 infected person. We show that allowing for mutation and extinction reduces strain diversity compared with deterministic models, with a strain carrying capacity set by cross-immunity and population size. The new model confirms the earlier results of simulations that reproducing influenza evolution requires models to incorporate a transient strain-transcending immunity. We also show that such models are able to reproduce the antigenic clustering of strains reported in recent work on the antigenic mapping of influenza.

Neil Ferguson and Pavlo Minayev

IC/MP668/121: Mathematical modelling of malaria and other vector-borne diseases.

Organiser: Nakul Chitnis (Swiss Tropical Institute, Switzerland)
Co-organiser: Melissa Penny (Swiss Tropical Institute and Universität Basel, Switzerland)

Vector-borne diseases, such as malaria and dengue fever, kill over a million people per year. The mathematical modelling of vector-borne diseases began in 1911 with Ronald Ross's basic compartmental-model, calculating a stability index to measure the level of malaria transmission. Since then, numerous mathematical models of disease transmission and immunology have been developed and analysed to assist the development and implementation of medicines, vaccines, and intervention strategies. In this minisymposium, we present a history of these models, what the current status of vector-borne disease modelling is, and where modelling can provide useful information to the medical and public health community. We examine some current efforts to model the dynamics of the malaria parasite within the human host, including the development of human immunity and the parasite's dynamics to evade immunity. We present a model of the mosquito feeding cycle that includes the effects of various intervention strategies that either reduce the mosquito-biting rate on humans or kill mosquitoes. We finally present a model of the interaction between malaria prevalence and the evolution of sickle-cell anaemia. These mathematical models provide us with a better understanding of disease dynamics, and can serve as important tools in helping to reduce disease morbidity and mortality.

Mathematical modeling of vector-borne diseases with applications to malaria and dengue fever. **James Hyman** (Los Alamos National Laboratory, USA), Gerardo Chowell (Los Alamos National Laboratory, USA), Nakul Chitnis (Swiss Tropical Institute, Switzerland) IC/MT4136/121

This talk will give an overview of the history, current status, and future directions of mathematical models for vector-borne diseases such as malaria and dengue fever. We describe sensitivity analyses on a mathematical model of disease transmission to determine the relative importance of model parameters to disease transmission and prevalence.

We will apply the models to analyze the impact of climatological variables on the incidences of the disease and will discuss the 2002 dengue epidemic in Colima, Mexico. We estimate the reproduction number from spatial epidemic data at the level of municipalities using a standard dengue epidemic model and assuming pure exponential initial epidemic growth and comparing this estimate fit to a more realistic epidemic model to the initial phase of the dengue epidemic curve. We compute sensitivity indices of the reproductive number (which measures initial disease transmission) and the endemic equilibrium point (which measures disease prevalence) to the parameters at the baseline values. For our malaria model, we find that in areas of low transmission, the reproductive number and the equilibrium fraction of infectious humans are most sensitive to the mosquito biting rate. In areas of high transmission, the reproductive number is again most sensitive to the mosquito biting rate, but the equilibrium fraction of infectious humans is most sensitive to the human recovery rate. This suggests strategies that target the mosquito biting rate (such as the use of insecticide-treated bed nets and indoor residual spraying) and those that target the human recovery rate (such as the prompt diagnosis and treatment of infectious individuals) can be successful in controlling malaria.

A mathematical model of malaria parasite dynamics within host. **Melissa Penny** (Swiss Tropical Institute and Universität Basel, Switzerland) IC/MT1909/121

A discussion and mathematical model of the dynamics of *Plasmodium falciparum* malaria infections within a host will be presented. The parasite's mechanisms of replication, antigenic variation and immune evasion, as well as the host's immune responses will be discussed. A discrete-time, stochastic model capturing these dynamics of an infection will be presented. The model considers current views of *Plasmodium falciparum*'s mechanisms of antigenic variation and captures the recrudescences seen in a typical human infection. The model also allows for drug treatment with the view to evaluate treatment regimes or possible vaccines in larger scale population models. Preliminary results and validation of the model will also be presented.

A mathematical model for the dynamics of malaria in mosquitoes feeding on a heterogeneous host population. **Nakul Chitnis** (Swiss Tropical Institute, Switzerland), Thomas Smith (Swiss Tropical Institute, Switzerland), Richard Steketee (PATH-Europe, France) IC/MT1884/121

We describe and develop a difference equation model for the dynamics of malaria in a mosquito population feeding on, infecting, and getting infected from a heterogeneous population of hosts. Using the force of infection from different classes of humans to mosquitoes as parameters, we evaluate a number of derived parameters, that can be compared to field data, that measure malaria transmission levels. By assigning different types of vector control interventions to different classes of humans, and evaluating the corresponding levels of malaria transmission, we can compare the effectiveness of these interventions. We show a numerical example of the effects of increasing coverage of insecticide-treated bed nets in a human population where the predominant malaria vector is *Anopheles gambiae*.

Coupling ecology and evolution: malaria and the S-gene across time scales. **Zhilan Feng** (Purdue University, USA) IC/MT1915/121

Malaria has long been a scourge to humans. The exceptionally high mortality of malaria in some regions has led to strong selection for resistance, even at the cost of increased risk of potentially fatal red blood cell deformities in some offspring. In particular, genes that confers resistance to malaria when they appear in heterozygous individuals are known to lead to sickle-cell anemia. Thus, there is balancing selection against the evolution of resistance, with the strength of that selection dependent upon malaria prevalence. Over longer time scales, the increased frequency of resistance in a population might be expected to decrease the frequency of malaria and reduce selection for resistance. However, possession of the sickle-cell gene leads to longer-lasting parasitaemia in heterozygote individuals, and therefore the presence of resistance may actually increase infection prevalence. We developed a model that explores the interplay among these processes. By coupling the dynamics of the epidemiology of malaria and the genetics of sickle-cell gene, our model allows for joint investigation of impact of malaria on the selection of S-gene and influence of genetic composition of a population on the maintenance of malaria. Our results are based on threshold conditions derived from the model by separating malaria disease dynamics on the fast time scale and the dynamics of S-gene on the slow time scale and by conducting stability analysis.

IC/MP329/122: Direct and inverse problems in channels and membranes.

Organiser: Martin Burger (Universität Münster, Germany)
Co-organiser: Heinz Engl (RICAM Linz, Austria)
Co-organiser: Robert Eisenberg (Rush Medical University, USA)

Transport through channels and membranes is of fundamental importance for biological function, since it is used to control many processes in health and disease. Various models have been developed in the last years in order to contribute to the understanding of channel function, which is of fundamental importance for controlling diseases and designing channels with specified function. In the mathematical community, this problem has received significant attention very recently, and poses various interesting challenges to modelling, analysis, computation, and, ultimatively requires the solution of inverse problems in order to determine their structure from the (electrophysiological) function.

The aim of this double mini-symposium is to provide an overview of recent developments in direct and inverse problems related to transport through channels and membranes. The first part will start with direct problems (modelling and simulation), while the second part will focus on inverse problems (identification of channel distributions in membranes, identification and optimal design of permanent charges in ion channels).

Inverse problems related to ion channels. **Kattrin Arning** (RICAM Linz, Austria), Lin He (RICAM Linz, Austria), Martin Burger (Universität Münster, Germany), Robert Eisenberg (Rush Medical University, USA), Heinz Engl (RICAM Linz, Austria), Marie Therese Wolfram (Universität Münster, Germany) IC/MT2343/122

Ion channels are proteins with a hole down their middle that allow ions to move across otherwise impermeable cell membranes, thereby controlling many important physiological functions, such as conducting electrical signals down nerve fibres and initiating muscle contraction.

Connecting two baths of fixed ionic concentrations, a single ion channel is immersed in hard-sphere fluid with charged ions. In 2002, Gillespie et al. simplified the movement of the ions to one dimension and described the particle transport as friction-limited drift-diffusion with all excess chemical potentials given by the density functional theory of Rosenfeld (1989, 1993). Furthermore, the applied local electrostatic potential and the fluxes of the different ionic species are modeled through the Poisson-Nernst-Planck (PNP) equations, a system of nonlinear PDEs.

Based on this model we investigate inverse problems related to ion channels. One important feature of the channels is their selectivity property, allowing only certain types of ions to pass. This selectivity is determined by channel structures such as permanent charge, channel geometry and confining potential. Based on measurments of output currents depending on different input voltages and bath concentrations we would like to identify these structural features using a simplified linearized PNP-model. As the underlying operator leads to an ill-posed problem, regularization techniques have to be applied. A second goal appart from the identification of the channel structure is the design of channels that show a desired behaviour such as particular selectivity properties. We also long to achieve this using inverse problems techniques with different regularization methods other than Tikhonov. As the solution of the nonlinear PDEs is quite a high computational effort, fast numerical algorithms will also be considered to speed up the solution of the inverse problem.

Direct and inverse problems in channels and membranes. **Robert Eisenberg** (Rush Medical University, USA) IC/MT2470/122

Channels control the movement of ions and electricity across membranes and cells and thus control an enormous range of biological function. The distribution of channels in different membranes of muscle fibers and the lens of the eye is a classical subject of electrophysiology studied in depth with impedance spectroscopy some decades ago without the benefit of the theory of inverse problems. Attention in the last decades has focused on the properties of channels themselves, particularly once they are open. Ions move through open channels by electrodiffusion and models of charge spheres are quite successful in analyzing and predicting biological function in the few channels studied to date. Extension to the thousands of channels of biological and medical interest requires efficient well designed experimentation because the experiments are so expensive. Solving the mathematical inverse problem of identifying channels will aid enormously. Improving the function of biological channels and building technologically useful channels are important future goals. Naive design will be much less efficient and successul than sophisticated design using the theory of inverse problems.

Density functional theory as a tool to study biological ion channels. **Roland Roth** (Max-Planck-Institut Stuttgart, Germany) IC/MT4792/122

Density functional theory of classical fluids provides a very powerful and general tool to study the free energy and the structure of confined fluids. Using density functional theory it is possible to study the behavior of ion channels, which are membrane spanning proteins.

In this talk a short introduction to density functional theory for a mixture of charged and uncharged spheres is given. We discuss what properties of the system can be calculated and how these calculations can be tested by the help of exact statistical mechanical sum rules. We show how results from relatively simple confining geometries can be generalized to a complex ion channel geometry by the help of the morphometric approach.

IC/MP329/122: Direct and inverse problems in channels and membranes. #2

Organiser: Martin Burger (Universität Münster, Germany)
Co-organiser: Heinz Engl (RICAM Linz, Austria)
Co-organiser: Robert Eisenberg (Rush Medical University, USA)

(For abstract, see session #1 above.)

Atomic structures of biological transmembrane pores as a basis for simulation of function. **Tilman Schirmer** (Universität Basel, Switzerland) IC/MT1223/000

Bacterial porins allow the passage of solutes across the outer bacterial membrane. Crystal structures show that the scaffold of the pore is a hollow beta-barrel constricted by inwardly folded loops that are forming part of the pore lining. The pore constriction of non-specific OmpF porin is highly charged and shows segregation of basic and acidic residues that face each other across the pore. A multitude of mutations have been analyzed functionally as well as structurally to get insight into the role of this peculiar charge constellation. Brownian dynamics simulations of ion translocation show good agreement with experimental cation/anion selectivity and relative single channel conductance[1]. The simulations reveal distinct trajectories for cations and anions due to the dipolar potential at the pore constriction. The pore seems to be optimised for high throughput and low selectivity.

The pore of the maltodextrin specific maltoporin (LamB) re-

veals an extended hydrophobic patch formed by six aromatic residues at the channel lining. As shown by X-ray crystallography maltodextrins bind to this *greasy slide* at the height of the channel constriction. The Conjugate Gradient Method has been employed to simulate the *register shift* of a maltohexaose sugar [2]. The results show that no large energy barriers have to be overcome, despite the presence of a multitude of protein-sugar hydrogen bonds.

[1] Phale, P.S., Philippsen, A., Widmer, C., Phale, V.P., Rosenbusch, J.P. and Schirmer, T.; Role of charged residues at the OmpF porin channel constriction probed by mutagenesis and simulation. Biochemistry 40, (2001) pp.6319–25.
[2] Dutzler, R., Schirmer, T., Karplus, M. and Fischer, S.; Translocation Mechanism of Long Sugar Chains across the Maltoporin Membrane Channel. Structure 10, (2002) p.1273.

Numerical approximation of solutions to nonlinear inverse problems. **Donald French** (University of Cincinnati, USA) IC/MT1750/122

Identification of detailed features of neuronal systems is an important challenge in the biosciences today. An interdisciplinary research team has been working to determine the distributions of ion channels in frog olfactory cilia. The cilia are tiny tube-like structures (0.2 microns in diameter) that extend from the olfactory receptor neurons. The first step in the transduction of an odor into an electrical signal occurs in the membranes of the cilia and is controlled primarily by the ion channels. A mathematical model involving integral and partial differential equations is derived to model experiments aimed at identifying features of the distribution of these ion channels. Numerical and analytical approximations to the model solutions are derived and used with experimental data to obtain estimates of the spatial distribution of the ion channels along the length of a cilium. The results from this mathematical and experimental study suggest that these channels have a non-uniform distribution.

Forward solvers for ion channels. **Marie Therese Wolfram** (Universität Münster, Germany) IC/MT2240/122

The main focus of our work is the mathematical description and numerical simulation of ion channels. A reasonable model are the so-called Poisson–Nernst–Planck (PNP) equations. We introduce a special linearization of the transient PNP equations, which leads to a mixed formulation. We briefly discuss the numerical aspects of such formulations, especially the use of low order Raviart–Thomas elements. Finally we illustrate our techniques with a 2D simulation of calcium selective ion channel.

A Poisson–Nernst–Planck model for biological ion channels: an asymptotic analysis in a 3-D narrow funnel. **Amit Singer** (Yale University, USA) IC/MT5038/122

We wish to predict ionic currents that flow through narrow protein channels of biological membranes in response to applied potential and concentration differences across the channel, when some features of channel structure are known. We propose to apply singular perturbation analysis to the coupled Poisson-Nernst-Planck equations, which are the basic continuum model of ionic permeation and semiconductor physics. In semiconductor physics the problem is a singular perturbation, because the ratio of the Debye length to the width of the channel is a very small parameter that multiplies the Laplacian term in the Poisson equation. In contrast to semiconductors, the atomic scale geometry of narrow ion channels sometimes makes this ratio a large parameter, which, surprisingly, renders the problem a singular perturbation in a different sense. We construct boundary layers and match them asymptotically across the different regions of the channel to derive good approximations for Fick's and Ohm's laws.

This is a joint work with John Norbury.

IC/MP405/122: Mathematics and mechanics in structural and functional biology: material modelling.

Organiser: Rolf Krause (Universität Bonn, Germany)
Co-organiser: Christian Hellmich (TU Wien, Austria)

Bones and soft tissues accommodate mechanical loading by distributing the biological material via interior and exterior growth in a somehow optimized manner.

The understanding and simulation of these processes is of great importance in many application areas as are surgery planing or the design of implants and prostheses. These biomechanical problems demand advanced interdisciplinary development upon a solid foundation of mathematics, mechanics, computing, engineering, and physical, chemical, and biological sciences. The aim of our minisymposia is to present and discuss in an interdisciplinary framework mechanical, mathematical, and computational tools in the area of structural and functional biology. One focus will be on the modeling of bones, including such phenomena as fracture healing. In the latter case different highly complex processes interact at different scales, from the molecular level over that where biological cells are observed, up to the macroscopic level apparent to the naked eye. These interactions are highly nonlinear, and their mathematical representation requires coupled multiscale and multiphysics models. The construction and analysis of efficient coupled models describing the mechanical properties of bone (and biological materials in general) as a result of ever changing biochemical cocktails provided through the well-tuned teamwork of biological cells (fibroblasts, osteoblasts, osteocytes, osteoclasts etc.) will be at the center of the talks and discussions in the proposed minisymposia.

Collagen fiber remodeling in arterial walls. **Ellen Kuhl** (TU Kaiserlautern, Germany) IC/MT2388/122

Functional adapation of biological tissues has advanced to a research topic of growing interest in the field of mechanobiology. The adaptation in response to mechanical loading can manifest itself in two fundamentally different forms: growth and remodeling. This contribution focusses on the latter with particular application to collagen fiber reorientation. A micromechanically motivated remodeling theory will be derived and applied to the adaptation of arterial microstructure which is known to remodel progressively to preserve circumferential wall stress and wall shear stress at a normal physiological level. Numerical examples will focus in partiular on the ongoing discussion whether stress or strain is the relevant quantity that drives the remodeling process.

Role of hydroxyapatite–collagen interactions on mechanics of collagen in human hard tissues. **Kalpana Katti** (North Dakota State University, USA), Dinesh Katti (North Dakota State University, USA), Rahul Bhowmik (North Dakota State University, USA) IC/MT3409/122

We have used structures of collagen-teliopeptide and hydroxyapatite to conduct molecular dynamics study to evaluate specific nature of hydroxyapatite-collagen interactions in human bones. The specific crystallographic planes of interaction of collagen with hydroxyapatite are identified. Further, we have also conducted a steered molecular dynamics study to evaluate the specific role of the bonded and non bonded interactions at the hydroxyapatite-collagen interface on the mechanics of the collagen. This study describes the role of molecular interactions during deformation in collagen while loading of bone.

Mechanics of mineral–protein interactions: a steered molecular-dynamics study. **Dinesh Katti** (North Dakota State University, USA) IC/MT3253/122

Hybrid interfaces are common in many structural biocomposites and nano-biocomposites. These mineral-organic hybrid interfaces and organic phase in biocomposites show unique mechanical behavior which many a times result in extraordinary properties exhibited by the bionanocomposite. In our current work, we focus on the aragonite-organic interface in a biological nanocomposite nacre, the shiny inner layer of seashells. Nacre which is a laminated biocomposite consisting of 95 to 98

Our previous work has shown the presence of platelet interlocks in nacre as key to the fracture toughness and strength in nacre (Katti etal. 2005). Our earlier work has also shown that the elastic modulus of organic phase which is predominantly proteins is exceptionally high (Katti etal. 1999, 2001). The organic phase has unique properties, very high elastic modulus and ability to deform considerably before failure. Recently we have shown that the mechanical response of proteins in the proximity of aragonite is significantly different from that of bulk proteins and shows some unique and distinct differences (Katti etal. 2005, 2006). The force required to unfold the protein in the proximity of aragonite is several times greater than the case in absence of the protein. In this work we describe our steered molecular dynamics simulations for studying aragonite-protein interactions and elucidate the mechanisms responsible for the extraordinary enhancement of mechanical response during protein unfolding in the proximity of aragonite.

Macro–micro characterization and modelling of human compact bone. **Marie-Christine Ho Ba Tho** (Université de Technologie Compiègne, France) IC/MT3586/122

The objectives of the present study were 1) to investigate the influence of multiscale structural characteristics of the bone tissue on its mechanical behavior and 2) to perform a macro-micro numerical modelling based on the experimental data. Ultrasound technique was used to assess the anisotropic behavior of cortical bone at the macrostructural level. Morphological measurements and mechanical testing were performed at that microstructural level. Morphological measurements were derived from ESEM images and mechanical testing consists of nanoindentation. In order to develop the mathematical model, variational approaches methods was used. From the knowledge of the mechanical characteristics of each constituent of the cortical bone at the microstructural level, variational approach to bound the elastic properties at the macroscopic level was used. The different steps of the mathematical modelling are 1) to describe the morphological patterns at the microstructural level, 2) to predict the effective elastic properties at the macroscopic level by the variational approach. The variation at the microstructural is related to the different degrees of maturation, mineralization of the osteons. The variation at the macrostructural level is related to microporosities of the cortical bone. Our mathematical model was validated by comparison between simulated results with that of the experimental data. Simulations allowed to quantify the effect of microporosities on the anisotropic behavior of bone, and effet of different morphological patterns on mechanical properties of bone. The mathematical model allowed the influence of the different patterns and their effect on the macroscopic anisotropic behaviour to be tested. One should note that in the first assumption of the isotropic behaviour of the mechanical properties at the microstructural level, one can predict the anisotropic elastic properties related to structural properties. Moreover, different possible structural and material configurations could be obtained for a same global macroscopic values. Other local distributions of patterns could be investigated reflecting bone pathology or else, then our model could be used to predict then global stresses, strain for such configuration. Conversely we emphasize the fact that, for a given global loading, the local strain or stress can be computed. For this point of view, one could estimate the local stresses inside the osteons. Moreover, investigations of the influence of the diameter of the Haversian canal and the size of the osteon lamellae could be performed. Finally, with the mathematical model, one can test the part of the structural and material anisotropy at the microstructural level on the macroscopic values. These simulations will provide a better understanding of the relationships between structural and material properties at different scale.

IC/MP405/122: Mathematics and mechanics in structural and functional biology: material modelling. #2

Organiser: Rolf Krause (Universität Bonn, Germany)
Co-organiser: Christian Hellmich (TU Wien, Austria)

(For abstract, see session #1 above.)

Universal micro-structural patterns in bone: continuum micro-mechanics-based prediction of anisotropic material behavior. **Christian Hellmich** (TU Wien, Austria), Andreas Fritsch (TU Wien, Austria) IC/MT3256/122

Bone materials are characterized by an astonishing variability and diversity. Still, because of ?architectural constraints?, their fundamental hierarchical organization or basic building plans remain largely unchanged during biological evolution. These building plans govern the mechanical interaction of the elementary components of bone (hydroxyapatite, collagen, water; with directly measurable tissue-independent elastic properties), which are here quantified through a multiscale homogenization scheme delivering effective elastic properties of bone materials: At a scale of 10nm, long cylindrical collagen molecules, attached to each other at their ends by 1.5nm long crosslinks and hosting intermolecular water inbetween, form a contiguous matrix called wet collagen. At a scale of several hundred nanometers, wet collagen and mineral crystal agglomerations interpenetrate each other, forming the mineralized fibril. At a scale of 5 microns, the solid bone matrix is represented as collagen fibril inclusions embedded in a foam of largely disordered (extrafibrillar) mineral crystals. Remarkably, needle and sphere type representations of disordered minerals deliver quasi-identical mechanical behavior of such extrafibrillar porous polycrystals. At a scale above the ultrastructure lacunae are embedded in extracellular bone matrix, forming the extravascular bone material. Model estimates predicted from tissue-specific composition data agree remarkably well with corresponding stiffness experiments across cortical and trabecular materials, which opens new possibilities in the

exploitation of computer tomographic data for nano-to-macro mechanics of bone organs, especially in combination with currently investigated extensions towards damage and failure.

Influence of tissue anisotropy versus inhomogeneity on the structural behaviour of an elderly human mandible. **Cornelia Kober** (FH Osnabrück, Germany), Christian Hellmich (TU Wien, Austria), Bodo Erdmann (Zuse-Institut Berlin, Germany) IC/MT2831/122

Within the biomechanics of bony organs, individual tissue anisotropy and inhomogeneity are intensively discussed subjects. This paper is dedicated to the impact of a fully anisotropic and inhomogoneous material description on the structural behaviour of an elderly partially edentulous human mandible.

Radial, axial, and circumferential trajectories of orthotropic elasticity were reconstructed from kind of inner skeleton derived from the organ's geometry and from coherent structures recognisable from the spatial distribution of the grey values coming from computer tomography (CT). Based on recent micromechanical research driven forward by the second author CT numbers were transferred into inhomogeneous stiffness tensor components reflecting individual tissue properties. These coefficients were considered as local orthoptropic elastic coefficients in reference to coordinate systems formed by the anisotropic trajectories of elasticity. For the sake of a complete anisotropic material description over the whole organ, the tensor components were transformed into a global base frame which allows assembling an overall patient-specific stiffness matrix.

Various sensitivity analysis revealed that the more the anisotropy is considered the more the mandible is spared from loading which indicates kind of mechanical optimality of the mandible with respect to tissue anisotropy. In the opposite, the consideration of individual inhomogeneous tissue properties resulted in intensification of load concentrations due to pathological alterations of the organ which gives rise to the suggestion of self-energising processes of bone resorption.

For the sake of reliability and efficiency, the numerical calculations were performed by means of the adaptive finite element code KASKADE, see www.zib.de/Numerik/numsoft/kaskade. The comparison of both the original (about 350.000 tetrahedra) and the refined mesh (about 800.000 tetrahedra) proved the simulation results as reliable.

Work done in collaboration with Stefan Stuebinger, Robert Sader and Hans-Florian Zeilhofer.

Universal morphological patterns in wood: micro-mechanics-based estimates for anisotropic stiffness and strength from composition and microstructure. **Karin Hofstetter** (TU Wien, Austria), Christian Hellmich (TU Wien, Austria), Josef Eberhardsteiner (TU Wien, Austria) IC/MT3299/122

Wood stiffness and strength are highly anisotropic. The material resistance in stem direction is about an order of magnitude higher than that orthogonal to the stem. Obviously, this anisotropy stems from the intrinsic structural hierarchy of the material. Wood is composed of wood cells, which are hollow tubes oriented in the stem direction. The cell wall is built up by stiff cellulose fibrils with crystalline cores and amorphous surfaces, which are embedded in a soft polymer matrix composed of hemicellulose, lignin, extractives, and water. The orientation of cellulose fibrils and tubular holes and the spatial gradation of porosity leads to anisotropy and inhomogeneity of the macroscopic material behavior.

The relation between (macroscopic) elastic material properties of wood and physical quantities at lower scales was recently expressed in the framework of continuum micromechanics. We here apply this model for estimation of the elastic properties of the wood cell wall, which are then related to macroscopic stiffness properties of wood by means of a unit cell approach. The latter allows for consideration of the plate-like bending and shear deformations of the wood cell walls, which are dominant at loading in the transverse direction. Model estimates for the elastic moduli and shear moduli of wood agree very well with corresponding experimental results.

Macroscopic material strength is governed by strain peaks in the material microstructure, which can be suitably characterized by quadratic strain averages over material phases, being effective for material phase failure. Macroscopic stress states estimated from local shear failure of lignin agree very well with corresponding strength experiments.

Analytical solution of crack problems in nacre. **Ko Okumura** (Ochanomizu University, Japan) IC/MT3301/122

Nacre is a remarkable nanoscale layered structure, which makes the beauty of pearl. This structure also contributes significantly to the unusual strength of this material. We show that the stress and strain distribution around a line crack in nacre, or similar layered structure, can be analytically obtained, in a certain mathematical limit relevant to nacre. The solutions reveal that the weakening of the stress concentration around the tip crack, which is one of the reasons of the unusual strength. We may also mention some scaling relations for fracture mechanical properties of natural cellular solids.

IC/MP4216/122: Mathematics and mechanics in structural and functional biology: simulation.

Organiser: Rolf Krause (Universität Bonn, Germany)
Co-organiser: Christian Hellmich (TU Wien, Austria)

Bones and soft tissues accommodate mechanical loading by distributing the biological material via interior and exterior growth in a somehow optimized manner.

The understanding and simulation of these processes is of great importance in many application areas as are surgery planing or the design of implants and prostheses. These biomechanical problems demand advanced interdisciplinary development upon a solid foundation of mathematics, mechanics, computing, engineering, and physical, chemical, and biological sciences. The aim of our minisymposia is to present and discuss in an interdisciplinary framework mechanical, mathematical, and computational tools in the area of structural and functional biology. The focus will be on the modelling and simulation of biological materials and their mechanical behavior. The construction and analysis of efficient solution methods for the arising coupled models will be at the center of the talks and discussions in the proposed minisymposia.

Analysis of nasal airflow phenomena using CFD simulations. **Stefan Zachow** (Zuse-Institut Berlin, Germany) IC/MT3560/122

Though treatment methods in ear, nose and throat surgery have constantly improved over time, the prediction of a successful individual therapy under consideration of regular nasal airflow remains a challenging task. Airflow simulations based on computational fluid dynamics are presented for a highly detailed anatomy of nasal airways, being reconstructed from tomographic data, including frontal and paranasal sinuses, naso-pharynx, and trachea. The simulation of complex airflow

characteristics with regard to individual anatomy enables us to study the physiology and pathophysiology of nasal breathing, thus being able to support treatment planning in functional rhinosurgery.

Efficient solution of non-smooth systems in biomechanics. **Rolf Krause** (Universität Bonn, Germany) IC/MT3145/122

Due to the inherent complexity of biomechanical systems, the solution of biomechanical problems in continuum mechanics is a challenging task. Understanding mechanical processes within, e.g. human joints or the spine requires carefull modelling and simulation, particularly in the case of multiscale models. In addition to the smooth nonlinearities, which might be induced by the material modelling, often constraints occur, e.g. for contact within joints. In this talk, we consider the influence of constraints and strong nonlinearities on the construction of discretizations and solutions methods in space and time in a biomechanical context. Different approaches are discussed and numerical examples and results are presented.

Cortical bone anisotropy due to mesoscopic porosity: investigations via asymptotic homogenization. **William Parnell** (University of Manchester, UK), Quentin Grimal (Université Pierre et Marie Curie, France), Pascal Laugier (Université Pierre et Marie Curie, France) IC/MT4394/122

A new model of cortical bone elasticity is developed and used to assess the influence of porosity on the macroscopic anisotropy of bone. In particular we use the method of asymptotic homogenization to determine the effective elastic properties of bone by modelling the propagation of low frequency elastic waves through the material. We use a novel solution of the cell problem developed by Parnell and Abrahams [1], [2] which is ideally suited to such a study due to its ability to model complex microstructure. Results, which are able to be computed efficiently (in seconds) are compared with existing homogenization and micromechanics schemes and finite element models from Grimal et. al. on real microstructures [3]. Parametric studies are performed in order to assess the influence of porosity and the assumptions regarding the constitutive behaviour of the material inside Haversian canals.

[1] Parnell, W.J. and Abrahams, I.D. (2006) Dynamic homogenization in periodic fibre reinforced media. Quasi-static limit for SH waves. Wave Motion, Vol. 43, pp 474-498.

[2] Parnell, W.J. and Abrahams, I.D. Homogenization for wave propagation in fibre reinforced media of complex microstructure. Submitted to J. Mech. Phys. Sol., January 2007.

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Apparent elastic properties of trabelcular bone. **Philippe Zysset** (TU Wien, Austria) IC/MT4988/122

Osteoporosis is a major health care issue in aging societies which is characterized by a reduction in bone mass and degradation of trabecular architecture leading to bone fractures. Using high resolution imaging technologies, the mechanical properties of trabecular bone can be simulated with classical or voxel-based finite element methods. As the computing resources required to simulate the mechanical behavior of whole bones or bone-implant systems with detailed trabecular architecture are prohibitive, the purpose of this study is to identify the most appropriate boundary conditions to calculate apparent properties of trabecular bone. Since the trabecular architecture exhibits nearly orthotropic symmetry, an artificial representative volume element is designed by mirroring the microstructure along the 3 orthogonal planes of symmetry. The effective elasticity tensors of artificial RVEs (10.4mm cubes) were computed with periodic boundary conditions (PBC) using a voxel based finite element method. Finally, kinematically uniform (KU), statically uniform (SU) and a novel set of mixed boundary conditions (BC) were applied to compute the apparent properties of the initial volume elements (5.2mm cubes). The KUBC leaded to an upper bound of the apparent elastic properties and overestimated significantly the effective properties of the mirrored volume calculated with PBC. The discrepancies increased with porosity and reached 400As a major result, the apparent elasticity tensors calculated with the novel set of mixed BC were nearly identical to the effective properties of the mirrored volume calculated with periodic BC. This novel set of mixed boundary conditions represents therefore an improved alternative to previous methods to compute realistic apparent elastic properties of trabecular bone.

IC/MP211/122: Stochastic biochemical systems.

Organiser: Peter Thomas (Case Western Reserve University, USA)
Co-organiser: Hong Qian (University of Washington, USA)

The chemical reactions by which living cells sense, control and respond to internal and external conditions typically involve small numbers of individual reactants. The stochastic nature of chemical reactions means that on the cellular or subcellular scale traditional methods of continuum, concentration based, chemical dynamics overlook essential phenomena. Reaction networks must overcome fluctuations as they attempt to maintain homeostasis or identify external signals, but they may also exploit noise to enhance stability or create movement. Topics to be discussed include fluctuations in cell motility, cellular communications and the statistical thermodynamics of open systems.

Mesoscopic and macroscopic open-system chemical dynamics. **Hong Qian** (University of Washington, USA) IC/MT3958/122

Chemical master equation (i.e., a birth-death process with continuous time), has become the mathematical foundation of chemical reaction kinetics in both small and large systems. In this talk, I shall discuss the unifying theory that encompasses both stochastic models and deterministic nonlinear chemical scillations. The essential difference between open and closed systems in terms of the "chemical detailed balance" will be discussed. The dynamic consequences of open-systems and their specific biological functions will be presented. For more information, see
http://dx.doi.org/10.1021/jp061858z,
http://dx.doi.org/10.1146/annurev.physchem.58.032806.104550.

Stochastic aspects of actin filament dynamics. **Hans Othmer** (University of Minnesota, USA) IC/MT4694/122

Actin polymerization and network formation are key processes in cell motility. Numerous actin binding proteins controlling the dynamic properties of actin networks have been studied and models such as the dendritic nucleation scheme have been proposed for the functional integration of at least a minimal set of such regulatory proteins. In this talk we will describe recent work on the evolution of the distribution of filament lengths and nucleotide profiles of actin filaments. The distributional dynamics of actin filaments are investigated in the framework of both deterministic and stochastic chemical kinetics. For the latter we develop a master equation for the biochemical processes involved at the individual filament level and simulate the dynamics by generating numerical realizations using a Monte Carlo scheme. A new computational algorithm that is far more efficient than standard methods will also be described.

Information-theoretic analysis of eukaryotic gradient sensing. **Peter Thomas** (Case Western Reserve University, USA) IC/MT4400/122

Chemical reaction networks by which individual cells gather and process information about their chemical environments have been dubbed "signal transduction" networks. Despite this suggestive terminology, there have been few attempts to analyze chemical signaling systems with the quantitative tools of information theory. Gradient sensing in the social amoeba *Dictyostelium discoideum* is a well characterized signal transduction system in which a cell estimates the direction of a source of diffusing chemoattractant molecules based on the spatiotemporal sequence of ligand-receptor binding events at the cell membrane. Using explicit Monte Carlo methods (MCell) we construct a simulation in which a collection of individual ligand particles undergoing Brownian diffusion in a three-dimensional volume interact with receptors on the surface of a static amoeboid cell. Adapting a method for estimation of spike train entropies described by Victor (originally due to Kozachenko and Leonenko), we estimate lower bounds on the mutual information between the transmitted signal (direction of ligand source) and the received signal (spatiotemporal pattern of receptor binding/unbinding events). Hence we provide a quantitative framework for addressing the question: how much could the cell know, and when could it know it? We show that the time course of the mutual information between the cell's surface receptors and the (unknown) gradient direction is consistent with experimentally measured cellular response times. We find that the acquisition of directional information depends strongly on the time constant at which the intracellular response is filtered; the equilibrium mutual information between the stimulus direction and the receptor states grows monotonically with larger time constants. However, for mean signal concentrations exceeding the equilibrium constant of the receptor, the mutual information peaks shortly after stimulus onset, suggesting that under some conditions cells should be expected to make directional decisions based on the transient receptor signal rather than on the long-time equilibrium signal.

Stability and robustness of synthetic band-pass response networks. **Attila Becskei** (Universität Zürich, Switzerland) IC/MT4998/122

Response to specified range of signalling intensity can be achieved by band-pass response networks. In order to increase the reliability and resistance to fluctuations, we designed the simplest possible network that at the same time neutralizes fluctuations. A single component gene circuit when combined with appropriate promoter logic displays a surprising robustness because it maintains band-pass response for all possible parameter values. At the same time the output fluctuations are small because correlated fluctuations appear in activating and repressing parts of the signalling pathway, which cancel out when combined.

IC/MP62/122: Dynamics of cell membranes.

Organiser: Axel Voigt (FZ caesar, Germany)
Co-organiser: Qiang Du (Pennsylvania State University, USA)

Biomembranes are a mixture of many different types of lipidic and protein components, and their relative amounts and composition differ between functionally distinct domains. In equilibrium membranes and in particular vesicles have been investigated intensively using a curvature-elastic model. However today curvature is no longer seen as a passive consequence of cellular activity but an active means to create membrane domains and to organize centres for membrane trafficing. Membrane curvature is thus a prime player in growth, division and movement of cells.

Recent advancements in applied mathematics allow the simulation of dynamic evolution of vesicles, with multiple components under the influence of flow. The underlying model includes the interaction of liquid with the elastic membrane, phase seperation and coarsening of composition on the membrane and the geometric evolution of the membrane according to curvature effects. The problem is a highly nonlinear free bounday value problem for which various numerical methods have been developed including phase-field, level-set and immersed boundary methods.

Surface-phase separation and flow in models of multicomponent vessicles. **John Lowengrub** (University of California, Irvine, USA) IC/MT3249/122

We introduce and investigate numerically a thermodynamically-consistent simple model of a vesicle in which the interfacial surface contains multiple constitutive components (e.g. amphiphilic molecules). The model describes the nonlinear coupling among the flow, vesicle morphology and the evolution of the surface phases. We consider a version of the Helfrich model for fluid- like vesicle membranes. To solve the highly nonlinear, coupled system a new numerical method is developed. This method combines the immersed interface method to solve the flow equations, and the Laplace–Young jump conditions, with the level-set method to represent and evolve the interface and a non-stiff Eulerian algorithm to update the mass concentration on the drop interface. Results are presented for vesicles in an applied shear flow where an initially unstable mixture of the surface mass separates into distinct phases.

Instabilities of inhomogeneous lipidic membranes. **Martine Ben Amar** (École Normale Supérieure de Paris, France) IC/MT4082/122

Lipid bilayer membranes are formed of multiple lipids which may separate into coexisting liquid phases with distinct compositions and physical properties. In cell biology, microdomains called rafts are receiving increasing attention since they are believed to concentrate proteins that must interact with one another to carry out important cellular functions. Here, we investigate the relationship between the curvature elasticity and the line tension of domains and the resulting formation of particular patterns or membrane shapes. Starting from the standard Canham-Helfrich elastic model, we write the free energy of our membrane restricted to two domains in order to allow axi-symmetry. Conserved quantities like the surface area are imposed via Lagrange multipliers while the semi-permeability of the membrane induces a global osmotic

pressure. When this pressure is strong enough, the vesicle is stretched and each phase takes approximatively the shape of a spherical cap. In this limit, the bending elasticity is negligible except in places of high curvature, that is at the border between the two domains. We derive an asymptotic model and show that a two-domain vesicle exists for a set of parameters such that the order parameter defined by the line tension divided by the pressure times the vesicle size remains below a critical value. Above this value, the two domains separate and two homogeneous vesicles appear. Our model explains the budding of a raft phase by an osmotic shock or by insertion of proteins like PLA2. Another aspect of the membrane physics, more important from a biological point of view, concerns the fluidity of the membrane.The viscous properties of membranes have been less explored and most of the experimental or theoretical works concern the diffusion of particles. Here, we suggest to use the difference between the two viscosities of the domains to exhibit contour instabilities analogous to the Saffman-Taylor instability in viscous fingering. The hydrodynamics of the membrane has been established by Saffman in the case of diffusion. We adapt the Saffman model to an hydrodynamic flow induced by suction. We show that suction may induce a border instability in an inhomogeneous membrane, the number of contour oscillations being related to the contrast of viscosities. Our theoretical treatment is illustrated by the suction of the raft phase in an inhomogeneous vesicle by human blood HDL (High-density lipoproteins).

Dynamics and rheology of vesicle suspension. **Chaouqi Misbah** (Université Grenoble I, France) IC/MT4913/122

Vesicles under shear flow exhibit various dynamics: tank-treading (tt), tumbling (tb) and vacillating-breathing (vb). We present first an analytical theory about these dynamics. We show a direct bifurcation from tt to tb if $C_a \equiv \tau\dot{\gamma}$ is small enough (τ= vesicle relaxation time towards equilibrium shape, $\dot{\gamma}$=shear rate). At larger C_a the tb is preceded by the vb mode. For $C_a \gg 1$ the vb mode coexists with tb. We analyse rheology and find that the effective viscosity exhibits a minimum at $tt-tb$ and $tt-vb$ bifurcation points. We present numerical results from boundary integral formulation and a phase field model. We also discuss other features, such as migration in Poiseuille flow, and the behaviour close to a substrate.

Equilibrium and dynamics of biomembranes. **Ricardo Nochetto** (University of Maryland, USA), Miguel Sebastian Pauletti (University of Maryland, USA), Andrea Bonito (Univ. Maryland at College Park, USA) IC/MT5035/122

When lipid molecules are immersed in aqueous environment they aggregate spontaneously into 2 mono-molecular layers or (bio-)membranes that form an encapsulating bag called *vesicle*. This happens because lipids consist of a hydrophilic head group and a hydrophobic tail, which isolate itself in the interior of the membrane.

As a first approach, we have studied a model based on geometry assuming that the equilibrium shapes are the minimizers of the Willmore energy under area and volume constraints. In this context, the biomembrane is the preponderant factor influencing the shape of the vesicle. A gradient flow is established to reach these equilibrium shapes. Then, the effect of the inside (bulk) fluid is taken into account leading to more physical dynamics. The boundary conditions couple Stokes equations to the constrained Willmore force. Some fourth-order fully-nonlinear problems that arise are solved using an adaptive finite-element method.

IC/MP62/122: Dynamics of cell membranes. #2

Organiser: Axel Voigt (FZ caesar, Germany)
Co-organiser: Qiang Du (Pennsylvania State University, USA)

(For abstract, see session #1 above.)

Phase-field modeling and simulations of cell membranes. **Qiang Du** (Pennsylvania State University, USA) IC/MT155/122

In this talk, we report some of recent works with colleagues at Penn State on the phase field modeling and simulations of the vesicle membrane deformation under elastic bending energy and the interaction with background fluid flows and other external fields. We discuss the relations between the phase field model and the sharp interface limits. We also numerical simulations of membranes with various topology.

Modeling of multicomponent lipid vesicles. **Axel Voigt** (FZ caesar, Germany), Andreas Rätz (FZ caesar, Germany) IC/MT556/122

We derive a thermodynamical consistent model for the dynamics of lipid vesicles with multiple components. The model consists of a coupled system of a Cahn-Hilliard like equation for the concentration on the surface and a Willmore-flow like equation for the evolution of the surface under constraints on volume and surface area. We discuss different numerical approaches for this model (phase-field, level-set and parametric) and show numerical results demonstrating the strong interplay of composition and curvature.

A stochastic immersed-boundary method incorporating thermal fluctuations: toward modeling cellular micromechanics. **Paul Atzberger** (University of California, Santa Barbara, USA) IC/MT588/122

The mechanics of many cellular systems involve elastic structures which interact with a fluid, for example the outer cell membrane deforms during protrusions generated during motility and cell organelles such as the Golgi Apparatus and Mitochondria involve membranes which deform and bud vesicular and tubular structures during biological processes. Modeling, analyzing, and simulating the mechanics of such systems presents many mathematical challenges. The immersed boundary method is one modeling approach for such systems, and has been applied to many macroscopic biological problems, such as blood flow in the heart and lift generation in insect flight. At the length scales of cells and cell organelles, thermal fluctuations also become significant and must be taken into account. In this talk we discuss an extension of the immersed boundary method framework which incorporates thermal fluctuations through appropriate stochastic forcing terms in the fluid equations. This gives a system of stiff SPDE's for which standard numerical approaches perform poorly. We discuss a novel stochastic numerical method which exploits stochastic calculus to handle stiff features of the equations. We further show how this numerical method can be applied in practice to model the basic microscopic mechanics of polymers, polymer knots, membrane sheets, and vesicles. We also discuss work on modeling the dynamics of cellular membranes.

Dynamic instabilities in biological membranes. **Aurora Hernández-Machado** (Universitat de Barcelona, Spain) IC/MT941/122

We study pearling instabilities in biomimetic vesicles motivated by recent experiments. The pearling is induced by the anchoring of amphiphilic polymers. We use a phase-field model which reproduces both equilibrium and non-equilibrium shapes

IC/MP689/122: Computational medicine.

Organiser: Martin Weiser (Zuse-Institut Berlin, Germany)
Co-organiser: Peter Deuflhard (Zuse-Institut Berlin, Germany)

This minisymposium covers a broad range of scientific-computing applications in medicine, including cardiovascular flows, cardioelectric patterns, biomechanics and cancer treatment. The unifying theme is the use of PDE models for the biophysical and medical situation. The targets of the presented work range from fundamental understanding of physiological processes up to individual treatment design, and involve modelling as well as simulation and optimization.

A multiscale model of thermo-regulation in the cancer therapy regional hyperthermia. **Peter Deuflhard** (Zuse-Institut Berlin, Germany), Martin Weiser (Zuse-Institut Berlin, Germany) IC/MT2341/122

Regional hyperthermia with microwave radiation is a cancer therapy aiming at heating deeply seated tumors in order to make them more susceptible to an accompanying radio- or chemotherapy. In the standard case, diffusion and cooling by perfusion of arterial blood dominate the temperature distribution. The talk presents a multiscale perfusion model that introduces a hierarchical coupling between vessels of different size as well as a regional coupling between tissue areas (steal effect). This multiscale model is able to reproduce effects observed in clinical practice and offers new possibilities for optimizing individual treatment plans. Numerical results for clinical data are presented.

Towards efficient and reliable simulation of musculo-skeletal loading in the human knee. **Ralf Kornhuber** (Freie Universität Berlin, Germany), Oliver Sander (Freie Universität Berlin, Germany), Rolf Krause (Universität Bonn, Germany) IC/MT3287/122

A precise prediction of loads and forces within human joints would support surgical decisions and thus increase the overall success of hip and knee surgery procedures. However, preoperative in vivo measurements are hardly possible and credible numerical simulation is a demanding task. In this talk, we consider 3D finite element models of the human knee with patient-specific geometry and particularly concentrate on efficient and reliable solvers based on domain decomposition and monotone multigrid.

Contact in joints: on the stability of multi-level solution methods for biphasic materials. **Rolf Krause** (Universität Bonn, Germany) IC/MT3191/122

Biphasic materials are often employed for the modelling and the numerical simulation of articular cartilage within joints. In combination with frictional or frictionless contact, the numerical solution of the arising discrete non linear systems is a demanding task, in particular for realistic geometries. We consider the stability and efficiency of different multilevel approaches for the numerical solution of the resulting non-smooth systems. A multilevel method is derived which allows for the efficient solution of these non-linear systems, including nonlinearities as contact and friction. Numerical examples on problem specific geometries in three space dimensions are given.

Mechanism of IP_3 induced intracellular Ca^{2+} oscillations. **Martin Falcke** (Hahn-Meitner-Institut Berlin, Germany) IC/MT1442/122

Oscillations on cellular level can arise by several fundamentally different mechanisms. The whole cell or parts of it may represent an oscillatory medium with oscillatory local dynamics or global events may be initiated repetitively by non-periodic processes like repetitive wave initiation. The first mechanism implies regular interspike intervals (ISI) while the second one entails ISI distributions exhibiting a linear dependence of the standard deviation on the average ISI. We show that experimental results support the second mechanism.

That provides the frame for a theory of intracellular Ca^{2+} dynamics as a hierarchy of stochastic events and with probabilities to be determined by a new theory of intracellular Ca^{2+} oscillations. We present first results of this theory.

IC/MP689/122: Computational medicine. #2

Organiser: Martin Weiser (Zuse-Institut Berlin, Germany)
Co-organiser: Peter Deuflhard (Zuse-Institut Berlin, Germany)

(For abstract, see session #1 above.)

Cardiovascular flow modelling. **Alfio Quarteroni** (École Polytechnique Fédérale de Lausanne, Switzerland) IC/MT1422/122

In this talk I will present some recent advances on the modelling of the cardiovascular system, the simulation of physiopathological flow conditions, the control and optimisation of prosthetic operations.

Simulating the electrical activity in the atria with applications to radio-frequency ablation. **Aslak Tveito** (Simula Research Laboratory, Norway), Svein Linge (Simula Research Laboratory, Norway), Mary MacLachlan (Simula Research Laboratory, Norway), Glenn Lines (Simula Research Laboratory, Norway) IC/MT1676/122

Irregularities in the electrical activity of the atria reduce the efficiency of the heart muscle and reduce the patient's ability to continue normal physical activity. Such irregular wave-patterns can be cured by delivering radiofrequency energy to the heart muscle and thereby destroy arrhythmogenic foci. In order to do this, the physician has to understand the wave pattern. This is currently done by performing careful measurements of the electrical signals. Although such measurements provide important information about the wave pattern, it is reasonable to assume that further insight can be gained by combining the measurements with a simulator which may provide a much more detailed view of the wave pattern. It is the purpose of this talk to discuss how this process can be simulated by solving a system of partial differential equations modelling the electrical activity of the atria. In particular, we will discuss how to incorporate measured data into the simulator. Simplified examples will be provided combined with simulation results based on real 3D atrial data.

Adaptivity in space and time for reaction–diffusion systems in computational electro-cardiology. **Luca Pavarino** (Università degli Studi di Milano, Italy), Peter Deuflhard (Zuse-Institut Berlin, Germany), Piero Colli Franzone (Università degli Studi di Pavia, Italy), Jens Lang (TU Darmstadt, Germany), Bodo Erdmann (Zuse-Institut Berlin, Germany) IC/MT1726/122

Advanced multiscale models in computational electrocardiology offer a detailed representation of the heart bioelectrical activity, ranging from the microscopic description of ion channels of the cellular membrane to the macroscopic properties of anisotropic front propagation in the whole heart. The models considered here are the Monodomain or Bidomain tissue representation that includes orthotropic anisotropy and homogeneous or heterogeneous intrinsic membrane properties, described by either the simpler FitzHugh-Nagumo model or the more complex Luo-Rudy phase I model. Numerical simulations are based on the multilevel 3D code Kardos, which employs adaptive linearly implicit methods in time and adaptive finite elements in space. The simulation results show that the method accurately resolves the evolution of the intra- and extracellular potentials, gating variables and ion concentrations during the excitation, plateau and recovery phases of the heartbeat.

Numerical simulations of arterial plaque ruptures. **Anna Pandolfi** (Politecnico di Milano, Italy), Anna Ferrara (Politecnico di Milano, Italy) IC/MT2622/122

Atherosclerosis is a vascular disease characterized by accumulation of lipids, collagen, muscle fibers, macrophages, calcium and necrotic tissue in the vascular wall. Atherosclerotic plaque rupture is a common cause of acute myocardial infarction and unstable angina. *Vulnerable* plaques –non calcified eccentric plaques with a thinning fibrous cap, a large lipid pool, and macrophage infiltration– are prone to rupture at locations where the stress induced from biomechanical and haemodynamic forces exceeds the intrinsic strength of the material.

We present three-dimensional finite element models of damaged arteries, used to investigate the influence of the geometry and tissue properties on the plaque rupture. The plaque rupture can by caused by an external mechanical action (balloon angioplasty) or by a spontaneous fatigue process (pulse pressure).

We adopted two geometrical models, one based on a simplified geometry, the second reconstructed from a contiguous set of *in vitro* magnetic resonance images of a damaged artery. The simpler model is used to investigate the influence of the geometry and composition of the plaque on the results of balloon angioplasty. The more sophisticated model is used to evaluate quantitatively the stress distribution induced by the mechanical action in the arterial tissue.

The artery wall, composed by three layers (intima, media and adventitia), is discretized with tetrahedral finite elements. The material is modelled with the hyperelastic anisotropic model proposed by Holzapfel et al. [1]. The material properties are calibrated by fitting experimental data available in the literature. The physical interface between plaque and artery is modelled with cohesive elements, as well as the fracture surfaces induced by the mechanical action. The fracture surfaces, lying along solid elements boundaries, are explicitly introduced in the model only when the tensile strength of the material is reached.

Reference

[1] G. A. Holzapfel, T. C. Gasser, and R. W.Ogden. *A new constitutive framework for arterial wall mechanics and a comparative study of material models. Journal of Elasticity*, 61:1Ű–48, 2000.

IC/MP128/012: Modeling and parameter estimation for cardio-respiratory and metabolic control systems.

Organiser: Jerry Batzel (Universität Graz, Austria)
Co-organiser: Mostafa Bachar (Universität Graz, Austria)

This minisymposium focuses on modeling the complex control interactions of the human cardio-respiratory (CVRS) and metabolic control systems. Medical conditions related to these control systems are at the center of concern for health policy planning especially as the current population ages. These medical conditions include orthostatic intolerance in the elderly, increasing incidence of diabetes, and autonomic dysfunction due to diabetic neuropathy. Modeling efforts seek to develop better quantitative understanding of the complex interaction of various control loops leading to potential clinical applications. However model validation and in particular application of such models to the clinical setting face key hurdles due to the significant number of parameters involved in models that reflect physiological mechanisms together with the clinical constraint of generally non-invasive patient testing which generates a restrictive set of data from which parameters can be estimated. Furthermore, the inter-individual variation in a physiological system's inventory of control responses adds further complication to model application for diagnosis and treatment design. For this reason special emphasis is placed on discussing issues involved in model validation strategies, data acquisition, and strategies for applying reduce models for clinical use. These modeling problems represent an important challenge to current research. This challenge will be met through continuous advancement in mathematical and numerical methodologies together with new measurement techniques for minimally-invasive or non-invasive measurement of a wider range of physiological quantities as well as by the active interdisciplinary interaction of mathematicians, physiologists, and medical clinicians.

Stochastic modeling of the dynamics in heart-rate variability. **Susanne Ditlevsen** (Københavns Universitet, Denmark), Niels-Henrik Holstein-Rathlou (Københavns Universitet, Denmark), Jørgen Kanters (Københavns Universitet, Denmark) IC/MT2342/0

The isolated sinus node is a periodic oscillator, but the interaction between the sympathetic and the parasympathetic nervous system causes the output from the sinus node to fluctuate in an apparently random manner. The physiological mechanisms underlying the dynamic behavior of the heart rate remains unsettled.

Here we propose a stochastic model to quantify the variability. The goal is to characterize malignant arrythmias and other heart failures contrasted to healthy subjects through convenient stochastic processes modeling the dynamics of the potential governing the heart beat.

Subject specific parameters are estimated using a recently developed estimation procedure developed by us to make inference about the underlying process of the membrane potential from data of the interspike intervals in neurons.

Sensitivity analysis and their application in biomedical modeling. **Franz Kappel** (Universität Graz, Austria) IC/MT2928/0

In this talk we will demonstrate the important of classical sensitivity analysis and general sensitivity analysis in the development of global models for biomedical application. Two biomedical applications will be given, one in Glucose-Insulin control in Type 1 diabetes and a second one related to a large cardiovascular and respiratory system model. We will seek to demonstrate that the combined application of both forms of sensitivity analysis are important for the problem of identification of parameters for such large systems.

Evaluation of pancreas transplant function in patients with type-1 diabetes mellitus. **Mostafa Bachar** (Universität Graz, Austria) IC/MT2914/0

In this talk we describe a model of the Insulin-glucose system in regards to pancreas transplant function in patients with Type 1 Diabetes Mellitus. We discuss approaches to data acquisition and news experiments made over an extended time frame in order to identify the parameters and to estimate beta-cell mass using Kalaman filtering methods, classical sensitivity analysis and general sensitivity analysis.

Analyzing short-term cardiovascular-respiratory control mechanisms. **Jerry Batzel** (Universität Graz, Austria) IC/MT2923/0

In this talk we discuss the problem of studying the interaction of the cardiopulmonary and arterial baroreflex interactions in modulating the responses to various forms of short-term hypovolemia in the human cardiovascular-respiratory system. The end product of such research will be to have a model that can quantitatively describe the interaction of the main baroreflex control loops that are primarily involved in short-term control. We will discuss various potential forms of control interactions and a variety of experimental data that can be used to pinpoint the nature of these interactions. Sensitivity analysis and other strategies of model analysis will be applied to study the model and experimental design and issues involved in the person-to-person variation in the combination of these control interactions. A validated model that could reflect the wide spectrum of clinical data on short-term control impairment could aid in the understanding and treatment of acute hypovolemic stress.

IC/MP128/012: Modeling and parameter estimation for cardio-respiratory and metabolic control systems. #2

Organiser: Jerry Batzel (Universität Graz, Austria)
Co-organiser: Mostafa Bachar (Universität Graz, Austria)

(For abstract, see session #1 above.)

Estimating infant respiratory parameters. **Martin Fink** (University of Oxford, UK) IC/MT2948/0

In this talk we will discuss problems associated with estimating parameters important for evaluating infant respiratory control function. We will discuss a model of respiratory control and apply sensitivity analysis and other methods for evaluating which parameters are estimatable from typical data available in the clinical setting.

Quantitative sensitivity analysis for model assessment: mathematical models for blood pressure and flow regulation. **Hien Tran** (North Carolina State University, USA) IC/MT3126/0

Sensitivity analysis addresses the question of how particular model outputs vary as the model parameters are perturbed about some nominal values. This type of model analysis is important since it will make it possible to identify which parts of the complex model are being utilized and how. This information is very useful to mathematical modelers as it allows them to simplify or reduce model complexity. Finally, sensitivity analysis is also beneficial to experimentalists as part of their experimental design. In particular, data for which the model is sensitive would need further characterization, as opposed to data for which the model is relatively insensitive. In this talk, we will illustrate this type of sensitivity based model analysis on mathematical models for the blood pressure and flow regulation during postural change from sitting to standing. In our previous studies, a cardiovascular model was developed describing blood pressure and low, compliance, and resistance in the heart and systemic circulation. This closed-loop model includes 11 compartments and two submodels: (a) a cardiovascular model that can predict blood pressure and ow velocity during sitting and (b) a control model that can predict autonomic and cerebral regulatory mechanisms during the postural change from sitting to standing. For the sensitivity analysis studies, we focus on the steady-state problem (during sitting). Even with steady-state consideration, the mathematical model involves 48 parameters that need to be estimated from experimental data. However, sensitivity analysis showed that out of 48 parameters, only 10 parameters are sensitive to the physiological data. Furthermore, sensitivity analysis makes it possible to reduce the complexity of the mathematical model. Finally, we present validation results of the reduced order model against data that consist of arterial blood pressure measurements from the finger and cerebral arterial blood flow velocity measurements.

Heart-rate regulation during postural change from sitting to standing. **Mette Olufsen** (North Carolina State University, USA) IC/MT3176/0

During posture change from sitting to standing, blood pools in the lower extremities of the body, leading to a decrease in blood pressure in the upper body and the brain and an increase in blood pressure in the legs. In subjects with orthostatic intolerance, postural change may cause dizziness, lightheadedness, or even fainting. The exact function of the cardiovascular and respiratory regulatory mechanisms in response to such orthostatic stress is not well understood, and our work aims to develop mathematical models that can help describe these regulatory mechanisms in more detail. One of these regulatory factors is heart rate, which is increased during postural change from sitting to standing. Changes in heart rate are mediated partly due to parasympathetic withdrawal, partly from a delayed sympathetic activation, and partly from musclesympathetic stimulation. In this work we present a model that predicts heart rate regulation during sit-to stand. Key elements of the heart rate model include a time-delay between sympathetic and parasympathetic nervous responses and an impulse function that predicts the vestibular response accounting for subjectŠs physical preparation for standing. Based on these responses we predict chemical changes of noradrenaline and acetylcholine and use an integrate and fire model to predict heart rate. This model has been validated against data from groups of healthy young, healthy elderly, and hypertensive elderly subjects.

Cheyne–Stokes respiration with cardiovascular pathologies. **William Langford** (University of Guelph, Canada) IC/MT4587/0

This work presents a compartmental model of the human cardio-respiratory system, simulating the factors that determine the concentrations of carbon dioxide in the compartments of the cardiovascular system and the lungs. The parameter set on which a Hopf bifurcation gives rise to Cheyne-Stokes respiration (CSR) has been determined. The model predicts that the onset of CSR oscillations may result from an increase in any of: ventilation-perfusion ratio, feedback control gain, transport delay, left heart volume, lung congestion or cardiovascular efficiency. The model is employed to investigate the relationship between CSR and serious cardiovascular pathologies, such as congestive heart failure and encephalitis, as well as the effects of acclimatization to higher altitudes. In all cases, the model gives good agreement with medical observations.

IC/MP233/012: Tissue deformation and cell motility: a new frontier in cancer modeling.

Organiser: Didier Bresch (Université de Savoie, France)
Co-organiser: Thierry Colin (INRIA Futur Bordeaux, IMB, France)
Co-organiser: Emmanuel Grenier (École Normale Supérieure de Lyon, France)

Modeling tumor growth is one of the most challenging and complex issue of biomathematics. This session focuses on the design and validation of specific models of tissue deformation and cell motility. Such models combine mechanical aspects together with chemiotaxis and biochemical phenomena, and are of primary importance for the understanding of metastasis or local invasion.

Taxis equations and cell motility. **Radek Erban** (University of Oxford, UK) IC/MT4578/0

Motile cells sense their environment and can respond to it either by directed movement toward or away from a signal, which is called taxis, or by changing their speed of movement and/or frequency of turning, which is called kinesis, or by a combination of these. These behavioural responses of different cell types will be analyzed. The corresponding taxis (partial differential) equations will be derived and its consequences presented, e.g. we show how experimentally-measured statistics can be obtained from the taxis equations.

Modelling and simulations of fibrous biological tissues via discrete homogeneization methods. **Vuk Milišić** (Université Grenoble I, France) IC/MT4762/0

Thanks to their geometrical organization at the cell level, muscle fibers and soft biological tissues can be modelled from the mechanical point of view as multidimensional networks of elastic bars. The length of the bars is supposed to be small with respect to the size of the macroscopic medium. We introduce a detailed description of the overall structure accounting both for the tensions due to bars and for the moments between pairs of bars. Using quasi-periodicity hypotheses, we apply a discrete homogenization technique, see [Caillerie, D. and Mourad, A. and Raoult, A., J. Elasticity, 2006]. This allows to pass to the limit when the size of the bars goes to 0. In such a way we derive a continuous homogenized mechanical law in the large transformation setting which has the structure of a membrane law. The expression of the stress tensor in terms of the deformation gradient is implicit. It involves an intermediate problem at the elementary brick level. This problem whose unknown are ordinary vectors is solved by means of an iterative method. We describe the basic principles of this approach that was first introduced in the cardiac modeling context in [Mourad, A. Phd thesis]. In a second step, we consider stability issues w.r.t. to the type of elastic energy used for bars and the corresponding parameters' values. In a last step we present its implementation in a finite element framework. We illustrate our method with numerical results related to mechanical behaviour of cardiac muscle fibers in 3D.

Mechanical models of tumour growth. **Luigi Preziosi** (Politecnico di Torino, Italy) IC/MT4492/0

The talk will deal with the multiphase framework recently developed to describe tumor growth. In particular the second part of the talk will focus on the potential role that stress responsiveness may play in causing proliferative disorders which are at the basis of the development of avascular tumours. We in fact study how an incorrect sensing of its compression state by a cell population can represent a clonal advantage and can generate hyperplasia and tumour growth with well known characteristics such as compression of the tissue, structural changes in the extracellular matrix, change in the percentage of cell type (normal or abnormal), extracellular matrix and extracellular liquid. A spatially independent description of the phenomenon is given initially by a system of nonlinear ordinary di erential equations which is explicitly solved in some cases of biological interest showing a first phase in which some abnormal cells simply replace the normal ones, a second phase in which the hyper-proliferation of the abnormal cells causes a progressive compression within the tissue itself, and a third phase in which the tissue reaches a compressed state, which presses on the surrounding environment. The space-dependent evolution in a two-dimensional set-up is then described numerically.

A mathematical model for tumor growth. **Olivier Saut** (Université de Bordeaux 1, France), Didier Bresch (Université de Savoie, France), Thierry Colin (INRIA Futur Bordeaux, IMB, France), Emmanuel Grenier (École Normale Supérieure de Lyon, France), Benjamin Ribba (Université Claude Bernard Lyon I, France) IC/MT4473/0

We present a multi-scale model of avascular tumor growth. This model takes the cell-cycle into account and several environmental conditions which could affect tumor growth (namely hypoxia, overcrowding).

For this matter, we describe the evolution of the proliferative and quiescent phases through several PDEs. The environment appears as a source term and as boundary conditions in these equations. To model hypoxia, we also have to compute the evolution of the oxygen distribution through a diffusion equation.

Furthermore, through a level-set formulation, this model can render the mechanical effects of an elastic membrane surrounding the cancer cells. This membrane is also degraded by tumor cells.

The velocity of the movement created by the cellular division (and the corresponding increase of volume) is obtained as solution of a Stokes equations. The elastic force due to the membrane we have just mentioned appears as a source term in these equations (and is vanishing outside the smoothed interface).

We also present the numerical methods used to discretize this model in three dimensions. With these numerical schemes, we show various numerical experiments highlighting the accuracy of the model. Finally, we will describe several extensions (*e.g.* angiogenesis) and applications to therapeutical innovation.

IC/MP591/123: Modelling cancer growth and treatment.

Organiser: Thomas Hillen (University of Alberta, Canada)
Co-organiser: Herb Freedman (University of Alberta, Canada)

This minisymposium consists of four talks related to the modelling of the growth and treatment of cancer and its dynamical relations to healthy cells. Most of the modelling involves ordinary, partial and functional differential equations. Each speaker will address one or more aspects of growth modelling and/or treatment, including a survey of models involving competition between healthy and cancer cells.

The tumor control probability in radiation treatment. **Thomas Hillen** (University of Alberta, Canada) IC/MT5041/123

The Tumor Control Probability (TCP) is an index that measures the expected success of a given radiation treatment schedule. The literature provides various models for the TCP, where the best known are the binomial and the Poissonian models, which are based on the LQ-formalism (linear quadratic model).

Through the fast developments in clinical studies, more and more detailed information becomes available and we should look into more detailed models for the TCP that can include current new insights. In 2000, Zaider and Minerbo developed a TCP model that includes the exact time course of the treatment. Dawson and Hillen extended this model to include cell cycle dynamics, since it is known that quiescent cells are less radio sensitive than proliferating cells.

In my talk I will explain all these models and compare their predictions. I will use the TCP models to compare 10 different treatment schedules including hypo- and hyper-fractionation schedules. (Joint with A. Dawson, O. Yurtseven, G. de Vries).

Mathematical modelling of radio-therapy: treatment success and hazards. **Heiko Enderling** (Tufts University, USA) IC/MT1861/123

When local treatment of breast cancer moved away from mastectomy to the less radical lumpectomy, it was realized that radiotherapy was essential to reduce local recurrence rates. The need to irradiate the whole breast after breast conserving surgery for early breast cancer, however, is currently being questioned and new radiotherapy schedules and techniques are being tested in clinical trials. Furthermore, recent trials aim to simplify radiotherapy by delivering fewer, larger fractions without compromising effectiveness. It may be possible to predict the results of these trials using sophisticated mathematical models, which incorporate new molecular oncology data, to capture the tumour dynamics and treatment response. We have created a mathematical model that simulates successively, the development, growth and invasion of a solid tumour within the breast; recurrence after surgery and the effect of radiotherapy. We will examine a range of current and prospective irradiation protocols that give the best chance for treatment success and minimize patient inconvenience. Additionally, we discuss the potentially hazardous side effects of new irradiation protocols with higher individual doses delivered in fewer fractions, as well as low dose screening protocols that are aimed at detecting breast cancer early.

Hypertumors in malignant neoplasia can be caused by tumor phosphorus demand. **John Nagy** (Scottsdale Community College, USA) IC/MT2007/123

In cancer, tumoral and peritumoral environmental conditions are controlled mostly by the unusual metabolism of malignant cells. Cancer cells are very metabolically active, and so require large amounts of reduced carbon, supplied as glucose. In addition, tumor cells need certain chemical elements for structural molecules. For example, tumors typically demand much more phosphorus (P) than normal tissue does, primarily because tumor cells upregulate ribosome biogenesis, which requires P. Because the body attempts to maintain homeostasis only in support of normal tissue function, tumors deplete resources locally in the short term. In the long term the depletion can become systemic, ultimately leading to cachexia, the most common cause of death in cancer victims. Here I use mathematical models to show that this unusual demand for P can lead to a hypertumor, which is a region of highly aggressive cells that grows parasitically on the original tumor and can kill all or part of it. Previous work has suggested that hypertumors may develop when a tumor is invaded by an aggressive cell type that fails to secrete angiogenesis factors. In this talk I introduce an entirely different mechanism of hypertumor development. In this case, the aggressive strain depletes P in the tumor interstitium, causing a decline in tumor growth rate or, in some cases, necrosis. If the tumor is large, this increased P demand speeds the patient towards cachexia. So, a hypertumor's effect both locally and systemically depends on the physiological state of the host and the developmental stage in which the hypertumor arises.

Motility and growth of cells as seen through the eyes of the Fisher–Kolmogorov equation. **Peter Hinow** (Vanderbilt University, USA), Glenn Webb (Vanderbilt University, USA) IC/MT5042/123

Transforming growth factor (TGF) β is a signaling molecule involved in a variety of cellular processes including growth, differentiation, apoptosis and cell motility. While TGF-β slows proliferation of certain cell types it also increases their motility and may decrease cell-cell adhesion. Thus, it has properties of both a tumor suppressor and a tumor promoting factor. We have carried out experiments to quantify cell motility and growth in presence of TGF-β and use a version of the classical Fisher–Kolmogorov equation to interpret the experimental findings.

This is joint work with Shizhen Wang, Nicole Bryce (Department of Cancer Biology) and Glenn F. Webb (Department of Mathematics, Vanderbilt University).

IC/MP189/124: New research in bioinformatics.

Organiser: Conrad Burden (Australian National University)
Co-organiser: Susan Wilson (Australian National University)

Bioinformatics is a rapidly growing interdisciplinary field concerned with the use of computational methods to solve biological problems related to DNA and amino acid sequence information. This minisymposium presents recent research from a broadly representative range of subfields within bioinformatics, namely 1. Comparative genomics: the comparison of DNA and amino acid sequences to identify evolutionarily related segments; 2. Gene regulatory networks: understanding how genes interact to control protein production through complex networks; 3. Protein structure: determining the geometric structure of protein molecules and 4. Microarrays: developing accurate high throughput technology for measuring gene expression within cells.

Asymptotic behaviour and optimal word size for exact and approximate word matches between random sequences. **Sylvain Forêt** (Australian National University), Conrad Burden (Australian National University), Susan Wilson (Australian National University), Ruth Kantorovitz (Univ. of Illinois at Urbana-Champaign, USA) IC/MT1801/124

A simple and efficient way of comparing two sequences is to count the number of words of length k letters (k-words) that they have in common. This number, D_2, has been used for the clustering of large collections of EST sequences. One of the main advantages of sequence comparison using D_2 is its speed, the runtime being proportional to the size of the sequence under scrutiny. In contrast, alignment-based comparisons have a worst-case run time proportional to the square of the size. The rigorous study of the statistical distribution of D_2, has been an active area of research and asymptotic regimes of this statistic have been derived. Progress has also been made in the characterization of the distribution of approximate k-word matches.

In an effort to test the applicability of these recent theoretical advances to real data, we computed the D_2 optimal word size for various sequence lengths, for both perfect and approximate word matches. Kolmogorov-Smirnov tests indicate that D_2 has a compound Poisson distribution at the optimal word size for small sequence lengths (below 400 letters) and a normal distribution at the optimal word size for large sequence lengths (above 1600 letters). We find that the D_2 statistic outperforms BLAST in the comparison of artificially evolved sequences, and performs similarly to other methods based on exact word matches. These results, obtained with randomly generated sequences, are also valid for sequences derived from human genomic DNA. In most cases, the best trade-off between computational efficiency and accuracy is obtained with exact word matches. Given that our numerical tests have not included sequence shuffling, transposition or splicing, the improvements over existing methods reported here underestimate what may be expected for real sequences. Because of the linear run time and of the known normal asymptotic behaviour, D_2-based methods are most appropriate for large genomic sequences.

Qualitative response of interaction networks: application to the validation of biological models. **Anne Siegel** (IRISA Rennes, France), Michel Le Borgne (IRISA Rennes, France), Ovidiu Radulescu (IRISA Rennes, France), Carito Guziolowski (IRISA Rennes, France), Philippe Veber (IRISA Rennes, France) IC/MT1792/124

We advocate the use of qualitative models for the analysis of shift equilibria in large biological systems. We present a mathematical method, allowing qualitative predictions to be made of the behaviour of a biological system. These predictions are not dependent on specific values of the kinetic constants. We show how these methods can be used to improve understanding of a complex regulatory system.

More precisely, a biological system is modelled as an interaction graph that can be built from databases or directly extracted from the literature. Based on the above mathematical framework, we derive a large system of qualitative equations which is translated into a system of polynomial equations on a Galois field. We use this method to assess coherency between the model and different types of data, and perform model/data correction. This approach also allows determination of hubs of the regulation network on behavioural grounds; that is, it enables determination of the products whose influence propagates through the network so as to maximally constrain the system response.

This approach is illustrated on the interaction network of *E. Coli* and on the network of genetic regulation in fatty acid metabolism.

Anisotropic atomic motion in proteins: comparison of experiment with theory. **Conrad Burden** (Australian National University), Aaron Oakley (Australian National University) IC/MT976/124

High resolution X-ray diffraction crystallography is now capable of resolving anisotropic atomic motions in biological macromolecules. This information is included in Protein Data Bank records in the form of anisotropic temperature factors. From a theoretical viewpoint, proteins are also studied with Molecular dynamics (MD) simulations using empirical force fields. In this work we compare anisotropic atomic fluctuations in nanosecond-timescale MD simulations with those observed in an ultra-high-resolution crystal structure of the crambin protein. In order to make our comparisons, we have developed a compact graphical technique for assessing agreement between spatial atomic distributions determined by MD simulations observed anisotropic temperature factors.

Natural metrics for gene-microarray calibration. **Hans Binder** (Universität Leipzig, Germany) IC/MT1260/124

A variety of array-based technologies have been developed to study the transcriptional architecture of the genome by estimating the expression degree or the copy number of selected genomic regions. Microarray experiments aim at measuring in parallel the abundance of thousands of RNA-transcripts or DNA-copies by optical detection of their sequence-specific binding to surface-grafted oligonucleotide probes. Current applications range from global analyses of transcriptional programmes of different organisms over the establishment of novel criteria for the classification and prognostics of diseases to the accelerated discovery of drug targets. The actual chip generation enables the very detailed genome-wide screening with several millions of probe spots on each exon, tiling and SNP (single nucleotide polymorphism) array. The raw intensity data of the probe spots are unfortunately affected by parasitic interferences which in many cases prohibit the direct translation of the intensities into the concentrations of specific target-fragments. The calibration of probe sequence related intensity variation is therefore a fundamental prerequisite for the analysis of oligonucleotide microarray data. Current methods rely on multichip normalization techniques and reference arrays. We report a new method of data adjustment which corrects raw microarray intensity data for the effect of (i) sequence-specific affinities; (ii) mismatches; (iii) cross-hybridization and (iv) saturation. The hybridization model describes specific and non-specific hybridization in terms of a competitive two-species Langmuir isotherm and the formation of probe/target duplexes in terms of positional dependent base-pair interactions. The approach is based on a physically-motivated metric system for GeneChip data which uses intrinsic relations between matched and mismatches probes. This single-chip method allows normalization of the intensities of each array without referencing with respect to other chips.

IC/MP9/125: Control of drug variability: drug-intake behaviour and beyond.

Organiser: Fahima Nekka (Université de Montréal, Canada)
Co-organiser: Jun Li (Université de Montréal, Canada)

Poor adherence to treatment is a worldwide problem of striking magnitude that threatens efficacy of therapy. This problem is of particular importance in the case of chronic diseases. The drug-intake behaviour has been shown to be a major determinant in therapeutic variability. Because of its random features, the adherence can be described using stochastic and statistical methods to quantity its effect for optimization of drug administration strategy or other impacts. This event is aimed to gather various visions and approaches for drug intake behaviour, in terms of data acquisition and processing. Delineating the different sources of variability induced by the dosage forms, their drug intake behaviour and drug response will be an issue.

Challenging problems in pharmacometrics related to drug-intake behaviour. **Fahima Nekka** (Université de Montréal, Canada) IC/MT2045/125

The adherence problem refers, in a generic meaning, to any misuse of the drug. It includes compliance, which refers to the quality of execution of prescribed drugs, and persistence, indicating the time lapse before discontinuation of the drug. The predicted therapeutic outcome to a well designed drug regimen is inevitably deviated by the drug intake behaviour. Compliance in human medicine has an analogue in veterinary practice when drugs are administered through feed. Indeed, livestock exhibit a great variability in their access to medicated feed. It is important to characterize the impact of this source of variability on different therapeutic outcomes. Using a stochastic approach, we have mathematically formulated drug-intake behaviour in population of animals to which a medicated feed is administered, which we integrated within a pharmacokinetic modeling process. Through simulation and analytical approach, we succeeded in delineating the impact of each feeding behaviour pattern, regular and random, in terms of the characteristic features of the drug-concentration time course. We have also developed a pharmacokinetic formalism explicitly integrating the patient drug compliance. We have decomposed the drug concentration expressions into a principal component, represented as an infusion process, on which is superimposed an oscillation component, the latter including multiple dose information for different administration routes along with patient compliance. We have shown that variable compliance adds additional variation to the oscillation curve that we properly characterized. We also proposed categorizing the impact of compliance into different levels, expressed through different statistical moments of the drug concentration.

Role of PBPK, PK-PD modeling in drug discovery: opportunities and limitations. **Thierry Lavé** (Hoffman-La Roche, Switzerland) IC/MT2110/125

During drug discovery, considerable resources are required to assess the pharmacokinetic properties of potential drug candidates in vivo in animals and there is interest in optimizing the use of such testing by applying simulation.

Physiologically based pharmacokinetic (PBPK) models take in vitro and in silico data inputs and can predict concentration versus time profiles before any in vivo experiment is performed. If sufficiently reliable, such simulations could decrease the turnaround time for delivery of information to medicinal chemists during the optimization phase and could also be used to prioritize compounds for the more costly in vivo testing. In addition, these models combined with the safety and efficacy properties of the compound can be used during early discovery to define the key parameters to be optimized in the context of the target profile of the compounds.

While pharmacokinetics in the rat is obviously not of ultimate interest for the pharmaceutical industry there is evidence that PBPK models are superior to other more empirical methods for interspecies scaling and prediction of human pharmacokinetics. Thus a verified PBPK model in rat can be scaled to human to provide a basis for the rational selection of compounds for clinical development and if combined with a pharmacodynamic model allows prediction of the efficacy profile in human. Equally importantly, the mechanistic framework provided by a PBPK model can integrate all available predictive data on a compound and provide mechanistic insights into compound properties. Such integrative capabilities and mechanistic insights are not provided by the more commonly used non compartmental or compartmental analysis.

The results on the use of generic simulation prior to in vivo studies indicate that some caution is required since certain chemical classes are poorly predicted and it is recommended that generic PBPK models should only be applied for prioritization after verification of the simulations with in vivo pharmacokinetics for a few compounds of a given chemical class. Such verification will help to identify invalid model assumptions or missing processes where additional data is needed.

There is growing evidence that PBPK-PD models can already add value at various stages of the pre-clinical compound research and development process although one has to keep in mind a number of limitations. Their use is growing and the potential will be fully exploited as powerful and user-friendly software continues to make PBPK-PD models accessible to non-specialists.

A physiologically-based pharmacokinetic model to assess the role of ABC. **Frederique Fenneteau** (Université de Montréal, Canada), Jun Li (Université de Montréal, Canada), Fahima Nekka (Université de Montréal, Canada) IC/MT4384/125

Background: Drug interactions affecting the expression and/or activity of ATP-Binding Cassette (ABC) transporters may have a significant impact on drug disposition, drug effectiveness or drug toxicity. Hence, the ability to accurately predict drug disposition over a wide range of conditions of ABC membrane transporter activities is required to better characterize drug pharmacokinetics and pharmacodynamics. The physiologically based pharmacokinetic (PBPK) modeling, considered as a well established methodology in the field of risk assessment and environment studies is now progressively used at variant stages of drug discovery and development.However, existing PBPK models have not been designed to characterize distribution of ABC transporters drug substrates in tissues, mainly because of the restricted access to ABC transporters-related physiological data and parameters. The most studied ABC membrane transporter is P-glycoprotein (P-gp), a multidrug resistance (MDR) protein found to be expressed in normal tissues, such as the intestine, kidneys, liver, brain, testis, ovaries, placenta, and heart. These numerous locations suggest an important role for P-gp in drug absorption and excretion and in limitation of drug penetration into target tissues. Objective: The objective of this study was to develop an innovative modeling approach that takes into account the involvement of ABC transporter activities in different tissues to improve the prediction accuracy of drug disposition. Method: A PBPK model was developed in order to consider various conditions of P-gp transporters activities in mouse brain, liver, kidney and heart tissues. Drug distribution was represented either by variants of well-stirred model or permeability rate limited model. Input parameters related to the activity of P-gp in theses tissues were mainly extrapolated from in vitro data. About 500 multivariate log-normal Monte-Carlo simulations were also performed to account for the variability of model parameters and their influence on the following output parameters obtained on each tissue: Cmax, Clast and AUC0-tlast. The measure of input-output sensitivity was performed using the partial rank correlation coefficient (PRCC) concept which has been designed for correlated inputs. Results: Our drug distribution models were successfully validated from experimental data collected on wild type and mdr1a/1b(-/-) mice which were intravenously administered 5mg/kg of 3H-domperidone. PBPK model simulations provided mechanistic information on the involvement of ad-

ditional membrane transporters in drug distribution.The sensitivity analysis based on Monte-Carlo simulations and PRCC concept showed that the AUC, Cmax and Clast values predicted in heart, brain, liver, kidneys and plasma are mainly affected by in vitro parameters: PappBA, Km , fup and Vmax. In brain and heart tissue, the value of efflux or influx clearance due to additional transporters activity have an important role in the variability of the output parameters. Conclusion: The herein described PBPK model is novel and unique, while defined in general terms that can be applied to other drugs and transporters.

A pharmacokinetic formalism explicitly integrating the patient drug compliance. **Jun Li** (Université de Montréal, Canada), Fahima Nekka (Université de Montréal, Canada) IC/MT4389/125

The adherence phenomenon is now well recognized to seriously compromise drug efficacy. In this paper, we analyze the role of compliance through drug intake history as an integral part of the pharmacokinetic process. Being concerned with what is accessible in medical practice, we develop a stochastic approach to model the drug intake behaviour that we combine with a conventional pharmacokinetics model in order to investigate the effect of drug intake history on the pharmacokinetic time-course. For this purpose, we explicitly formalize the plasma concentration variations for the most common administration routes. This analytical approach allows to characterize drug concentration variations directly inherited from patient compliance.

IC/MP185/015: Dynamical systems approaches in neuroscience: theory, experiments, and applications.

Organiser: Robert Kozma (University of Memphis, USA)
Co-organiser: Yuzuru Sato (Hokkaido University, Japan)

Dynamical aspects of neuroscience gained significant popularity in recent years. The accessibility of new experimental tools (fMRI, high-resolution EEG and MEG) provide us with very deep and unprecedented insight into brain functions at cellular, population, and macro levels. The observed neural mechanisms show a rich variety of complex and self-organizing dynamics between stimulus and response. Neural correlates of higher cognitive functions have been identified and described in details, but a comprehensive and rigorous theory of neural functions is still missing. The available experimental data represent a great challenge to mathematical modeling and analysis of brain processes. New nonlinear mathematical and computational models (e.g., pulse-coupled neural networks, spiking neuron models, large scale multi-component statistical simulation models, and others) were developed in recent years that can be employed to analyze, interpret and explain the available data. The goal of this mini-symposium is to create a forum for researchers on the exciting research area of mathematical methods and applications of neurodynamics. We will discuss recent developments, and also outline perspectives for future activities. Leading experts in the relevant research areas will contribute to the interdisciplinary topics of the mini-symposium. These may include the following areas: (i) theoretical aspects and modeling of neurodynamics using various mathematical tools, as nonlinear differential equations, coupled map lattices, random cellular automata, neuropercolation and random graphs, liquid state machines, dynamic neural networks; (ii) description and interpretation of experiments with neural systems, like cellular and population level mechanisms of learning and memory, adaptation, high level cognitive functions; (iii) application of dynamical neuroscience principles in the design and implementation of artificially intelligent systems, as embodied intentional robotics, robot cooperation, control, and autonomy.

Oscillatory cortical network dynamics. **Steven Bressler** (Florida Atlantic University, USA) IC/MT3772/015

The mammalian cerebral cortex is organized as a large-scale network of distributed areas, each with a specialized pattern of connectivity. It has been proposed that cognitive function depends on the dynamic coordination of activity in sets of interconnected areas. Experimental evidence suggests that this coordination occurs by the phase synchronization of neuronal population oscillatory activity in the beta (13-30 Hz) and gamma (30-100 Hz) frequency ranges. Phase-synchronized oscillatory networks in the beta frequency range, as measured by spectral coherence, have been shown to be organized with respect to motor maintenance and visual anticipation in the sensorimotor and visual regions of cortex, respectively. Furthermore, the phase synchronized oscillations have been found to carry influences between neuronal populations of the networks, as measured by spectral Granger causality. The theory and significance of oscillatory cortical network dynamics will be discussed.

Beyond odour coding: oscillatory and behavioral dynamics in olfactory perception. **Leslie Kay** (The University of Chicago, USA) IC/MT3724/015

One of the most striking features of olfactory system physiology is odor-evoked fast oscillations, which represent varying degrees of underlying neural precision and coherence. Recent studies have shown that artificial ablation (in insects) of fast oscillations impairs and artificial enhancement (in mice) of this measure of global precision enhances discrimination of similar odorants. The true test of whether fast oscillatory precision plays a functional role in odor discrimination depends on whether individuals manipulate the level of oscillatory activity online in a task-dependent fashion. We show that rats do this such that fast temporal precision (gamma oscillation power) is significantly enhanced in difficult odor discrimination tasks, while it is unaffected in easy discrimination tasks. At the low end of the frequency spectrum are theta band olfactory bulb oscillations associated with inhalation and afferent drive to mitral cells. This slow coupling among principal neurons, characterized by a burst-like firing pattern, is disrupted when rats sniff at higher frequencies. However, during fast sniffing in odor investigation significant coherence at high theta frequency is found between the olfactory bulb and hippocampus in a performance-dependent fashion. These two sets of results suggest that fast and slow cooperative activity can operate simultaneously to serve different purposes, fast precision facilitating formation and recall of neural assemblies within a sensory area and slower theta-band coherence facilitating interregional cooperation in sensorimotor integration. Both of these modes are adjusted dynamically to respond to task demands. (Funding NIDCD R01DC00795)

A novel method of control using chaotic dynamics in systems having many degrees-of-freedom. **Shigetoshi Nara** (Okayama University, Japan) IC/MT3449/015

Chaotic dynamics in systems having many degrees of freedom are investigated from the viewpoint of harnessing chaos and is applied to complex control problems to indicate that chaotic dynamics has potential capabilities for complex control functions by simple rule(s). An important point is that chaotic dynamics generated in these systems give us autonomous complex pattern dynamics itinerating through intermediate state points between embedded designed attractors in high-dimensional state space. A key point is an idea that, with the use of simple adaptive switching between a weakly chaotic regime and a strongly chaotic regime, complex problems can be solved. As an actual example, a two-dimensional maze, where it should be noted that the set context is one of typical ill-posed problems, is solved with the use of chaos in a recurrent neural network model. Our computer simulations show that the success rate over sevral hendreds trials is much better, at least, than that of a random number generator. Our functional simulations indicate that harnessing of chaos is one of essential ideas to approach mechnisms of brain functions.

Modeling scale-free cortical dynamics using neuro-percolation approach. **Robert Kozma** (University of Memphis, USA) IC/MT2474/015

Critical properties of dynamical models of neural populations are studied. Based on the classical work of Renyi-Erdos on the evolution of random graphs, a new class of random cellular automata models called neuropercolation has been introduced in the literature. We analyze the properties on the neuropercolation model of the neuropil, the densely connected tissue in the cortex. We show the emergence of phase transitions in neuropercolation models at critical combination of several control parameters, including the level of external gain and noise, the density of long-range axonal connections (small-world phenomenon), and the sparseness of feedback between excitatory and inhibitory neural populations. Noise level and structural properties of the cortical tissue has been used to control the critical exponent, starting from white noise (slope 0) far away from criticality. The results show that scale-free power spectral density characterizes the dynamics near criticality, where exponent with a power exponent approaching -2. The results are interpreted in the context of recent experimental findings on the dynamics and structure of the cortex.

12: Bio-Mathematics, Contributed Talks

IC/CTS4631/12: **Other medical applications.**

Organiser: Eamonn Gaffney (University of Oxford, UK)

On numerical study of 2D periodically-forced internal flows. **Corina Alexandra Olah** (Université de Nantes, France) IC/CT560/015

Periodically-driven flows occur in several important applications such as flows in the blood circulatory system, the respiratory system, industrial mixers, etc. Despite their practical interest, relatively few literature is available on periodically driven flows, and several questions remain open: Under what circumstances a viscous flow driven by periodic boundary conditions ceases to be periodic? Which sequence of bifurcations transforms a periodic periodically-driven flow into a fully turbulent flow?

Even more striking is the fact that the existence of a solution for the weak formulation of the time-periodically forced Navier–Stokes equations, no matter how small is the viscosity or how large is the Reynolds number, has been known for a long time [1]. But the unicity and stability of that periodic solution is not guaranteed by the theorem. Few attempts at looking at the stability of periodically-driven flows have been done [2,3,4,5]. Those few studies show that periodic periodically-driven flows become unstable while increasing the Reynolds number.

The purpose of my work is to introduce and study the stability of simple time-periodically driven flows with a forcing induced by boundary conditions and to investigate the first bifurcation in 2D laminar pulsating flows. Another aspect is the investigation of the speed of convergence to a time-periodic solution, in case the time-periodic solution is stable, with two main types of periodic forcing, tangential and normal forcing on the boundary. Numerical results are presented for periodically-driven flows in a square cavity and the critical Re, at which a bifurcation occurs, is identified. Then, the experiments extend to stenosis, where a time-periodic condition is imposed at the inflow, in order to assess the parameters controlling the convergence to a time-periodic solution. Also, the results of some 3D simulations will be presented.

Work done in collaboration with Prof. Yves Bourgault, University of Ottawa, ON, Canada.

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Numerical modeling of extra-corporeal shock-wave therapy. **Kirsten Fagnan** (University of Washington, USA), Randall LeVeque (University of Washington, USA) IC/CT830/125

Extracorporeal Shock Wave Therapy (ESWT) is a noninvasive technique for the treatment of a variety of musculoskeletal conditions such as delayed union of fractures, plantar fasciitis and calcified tendonitis of the shoulder. Shock waves were first used medically as lithotripsy (ESWL) to pulverize hardened calcified deposits such as kidney stones. The first application outside of lithotripsy was the treatment of calcifications in the shoulder since these deposits are similar to renal calculi. ESWT is also an effective treatment of non-unions, which are bone fractures that fail to heal over time. In lithotripsy, a shock wave is generated in a liquid bath, focused by a brass ellipsoidal reflector, and it then propagates into the body where it strikes the area of interest. Current numerical models are limited to simplified situations because the structure of the wave is highly nonlinear and therefore difficult to model with traditional finite difference and finite element techniques. We use high-resolution finite volume methods to capture this nonlinear behavior and model the shock wave propagation in bone and tissue by solving the nonlinear elasticity equations. This approach has been successfully applied to many problems in acoustic or elastic wave propagation in heterogeneous media.

We have obtained results in two- and three- dimensions by utilizing the CLAWPACK and CHOMBOCLAW software packages. CLAWPACK is a set of freely available Fortran routines de-

veloped by Randy LeVeque at the University of Washington. CHOMBOCLAW was written by Donna Calhoun as an extension of CHOMBO a freely available set of tools for solving equations using adaptive mesh refinement.

Mathematical and numerical modelling of focal ischemia. **Mauro Perego** (Politecnico di Milano, Italy) IC/CT4793/125

Relevance of a deep comprehension of the brain tissue damage mechanisms during focal ischemia has been realized since a long time. Besides the set up of therapies for stopping tissue degeneration in the ischemic penumbra, a possible outcome is the understanding of the failure of medical treatments that in other districts yield good results. For instance, fibrinolythic therapies, that works in the coronary districts, in the neurological context can lead to dangerous blood hemorrhages.

A possible approach for having a deeper insight of these phenomena is to resort to mathematical models and numerical simulations. The main difficulties in this context concern the intrinsic complexity of the phenomena and geometries at hand, that involve interacting fluid and biochemical dynamics, and the parameters identification and evaluation.

Numerical simulations presented in the literature are so far limited to 2D geometries and use a lumped average parameter to describe the cerebral blood flow, obeying an ordinary differential or an algebraic equation.

The aim of the present work is twofold. The first goal, is to give a rigorous model for the ions dynamics and include a space dependent description of the blood dynamics assuming that the vascular tissue is a porous medium. The second goal is to present numerical simulation of the phenomena at hand in 3D, by means of ad hoc finite element code.

The numerical results presented here show at a qualitative level possible dynamics that can be induced by the combination of biochemical events induced by the stroke and the reperfusion of the occluded vessels. The quantitative validation of the model used here is complicated by the difficulties in collecting experimental data. Nevertheless, it represents an important development of the present work.

Numerical simulations of low-energy defibrillation of the atria. **Monica Hanslien** (Simula Research Laboratory, Norway), Glenn Lines (Simula Research Laboratory, Norway), Joakim Sundnes (Simula Research Laboratory, Norway), Aslak Tveito (Simula Research Laboratory, Norway) IC/CT2239/125

Atrial fibrillation is the most common heart rhythm disorder, with possibly severe long-term complications for the patient. Strong electric shocks are known to cure fibrillation with high success rate, particularly those delivered by an implantable cardiodefibrillator (ICD). Although defibrillation has been subject to a great extent of research for many years, the phenomenon is yet poorly understood. We believe that numerical simulations can help understanding what is observed in medical experiments. Unfortunately, with today's technology and knowledge of defibrillation, the shock strength needed to terminate fibrillation is known to cause intolerable pain to the patient. Also, the recurrence of atrial fibrillation is frequently observed. It is therefore of the utmost interest to seek methods of intracardiac defibrillation that allows for lower shock strength, and to find the optimal placement and the number of electrodes used in the configurations.

We address these issues in the present talk. In particular we investigate the effect of such low-energy shocks on the atria, delivered through several electrode configurations, and of different strengths. We show results of bidomain simulations on a realistic geometry of the entire atria, using sophisticated numerical methods.

Modelling mucoiliary flows. **Eamonn Gaffney** (University of Oxford, UK) IC/CT2778/125

Mucociliary fluid flows are ubiquitous in nature, playing important roles in the lung, the ovaries and the ear. However, the quantitative details of such flows are poorly understood. In the lung cilia drive mucus towards the trachea. The cilia beat in a very thin, stratified liquid consisting of a basal Newtonian layer known as the periciliary fluid (PCL), and an upper mucus layer.

A model of mucociliary transport has been constructed which incorporates both mucus viscoelasticity and the effects of beating cilia. This provides, inter-alia, a physical basis for the observation in pseudo-hypoaldosteronism that excessive mucus hydration leads to increased mucus transport, via a thicker, less viscous, mucous layer. We have additionally demonstrated that empirical observations of microbead transport in in-vitro models of mucociliary flows need not correlate to the flow profile suggested by experimental scientists, due the effects of mixing and diffusion perpendicular to lung epithelium.

Work in collaboration with: DJ Smith, JR Blake.

IC/CTS4643/12: Modelling in bio-engineering.

Organiser: Diana Rubio (Universidad National de General Sarmiento, Argentina)

A 1D inverse problem with interfaces in bio-engineering. **Diana Rubio** (Universidad National de General Sarmiento, Argentina), María Troparevsky (Buenos Aires, Argentina) IC/CT3459/015

In this work we study a 1D Inverse Problem that is motivated by the electroencephalogram (EEG) problem, which consists in the use of EEG data to find the location of electric sources of neural activity in the brain. The problem is described by a Poisson type equation with interfaces, since the patient's head is modeled as nested layers. The elliptic equation has discontinuous coefficients due to the different conductivity values for the brain, skull and scalp.

In a previous work presented at ICNPAA 2006, a simple 1D model of the problem was considered to illustrate theoretical and numerical aspects of the computation of sensitivities. Here, we present some ideas to develop a numerical scheme to approximate the solution to the Inverse Problem for the 1D model for the case of a pointwise source. It is our intention to use these ideas to face the 3D Inverse Problem in a near future.

Multiple folding and packing in DNA modeling . **Francesca Maggioni** (Università degli Studi di Milano Bicocca, Italy), Renzo Ricca (Università degli Studi di Milano Bicocca, Italy) IC/CT3139/010

By using a new set of kinematic equations (see Maggioni & Ricca, *Proc. R. Soc.* A **462**, 2006) we study geometric and energetic aspects associated with multiple folding and coiling of elastic filaments for DNA modeling. By these equations we demonstrate that high degree of coiling may be achieved at relatively low energy costs through appropriate writhe and twist distribution, and independently from the number of coils formed. For sufficiently high twist we show that coiling is actually favoured by elastic energy relaxation, when the deformation energy is purely due to filament curvature and mean twist. We also determine the packing rate associated with filament compaction in the case of a hierarchical helical coiling. These results find useful applications in modeling DNA wrapping in proteic regions, where there is a strong connection between high coiling, efficient compaction and energy localization.

Wing disc size and robustness of Dpp gradients. **Frederic Wan** (UC Irvine, USA) IC/CT4235/015

A reaction-diffusion system of partial differential equations that accounts for the biological processes at work in the Drosophila wing imaginal disc essential for signaling decapentaplegic (Dpp) gradient formation is examine to investigate the effect of the epical-basal height of cells on the shape of signaling gradients. Our principal result is the relation between the epical-basal cell height and magnitude and shape of signaling Dpp gradient along the anterior-posterior axis of the wing imaginal discs. The result is used to delineate the effect of wing disc size in maintaining the shape of a normal signaling gradient and thereby the robustness of the normal development of the organism.

Acknowledgment: The research is supported in part by NIH grants P20GM66051 and R01GM067247. The research of Nie and Wan is also supported by NIH Grant R01GM075309. The two NIH R01 grants are awarded through the Joint NSF/NIGMS Initiative to Support Research in the Area of Mathematical Biology.

Understanding the anti-body mutation process by mathematical methods. **Lei Zhang** (Humboldt-Universität zu Berlin, Germany) IC/CT1423/124

A very important phenomenon observed in immunity is the antibody affinity maturation that leads to an efficient recognition of an invading pathogen during infection. Germinal centers are the major sites for antibody production, mutation and selection. In order to understand the underlying mechanisms during the mutation process, we developed simple mathematical models to analyze the available DNA sequence data derived from germinal centers (GCs) of the immunized mice. First, we calculated the frequencies of observed mutations in antibody sequences and compared them with theoretical predictions calculated from positional mutability and type of mutation. Our theoretical result not only confirmed the two known key mutations found experimentally, but also records 32 others positively selected mutations. This result suggests that an effective antibody binding may be a result of additive effects of positively selected mutations rather than a few large effects by key mutations. Also, we further identified 19 negatively selected mutations, which may represent harmful mutations whose harboring cells are eliminated rapidly by programmed cell death. Second, although it is not possible to follow the development of individual GCs by experimental means, mathematical modelling provides insights into the antibody maturation process in time. Our results suggest a much shorter history of mutation process in comparison with previous predictions. Such implications may change our current understanding on the underlying mechanisms of antibody mutation.

Stability analysis of a tritrophic food-chain model. **Jean Tchuenche** (University of Dar es Salaam, Tanzania) IC/CT35/121

The study of three-species communities have become the focus of considerable attention, and since ecological communities studies starts with its food web, we consider a tritrophic food chain mode comprised of the prey, the predator and the super-predator. The classical assumption of the domino effect is replaced by an adaptive parameter. Dynamical behaviours, boundedness, bifurcation, as well as stability are analyzed. Practical implications are explored and related to real populations.

Individual-based modelling of chlamydial infection. **Daniel Mallet** (Queensland University of Technology, Australia), Kel Sutton (Queensland University of Technology, Australia), David Wilson (University of New South Wales, Australia) IC/CT3208/012

Chlamydia is amongst the most common sexually transmitted diseases in the world and when left untreated, may lead to infertility and numerous other conditions. Currently, most mathematical modelling in the literature regarding Chlamydia is based on time dependent differential equations. In this work, we include spatiotemporal considerations of the progression of chlamydial infection in the genital tract. This novel direction is achieved using cellular automata modelling with probabilistic decision processes. In this presentation, the modelling strategy will be described, as well as its relationship with existing models and the advances in understanding that are achieved with such a model.

IC/CTS4638/12: Mathematical modelling in life sciences.

Organiser: Achim Schroll (Lund universitet, Sweden)

Spatio-angular modeling for the formation of oriented patches in chondrocytes cultures. **Viviana Palumberi** (Universität Basel, Switzerland) IC/CT4489/120

In cell therapy applications, the use of cytokines during cell expansion has been proposed as a promising method to increase the number of cells that can be obtained starting from a small tissue biopsy. In particular specific growth factors have been recently shown to enhance AHAC proliferation rate of adult human articular chondrocytes (AHAC) expanded in monolayer. We have recently developed a model combining time-lag (delay) and logistic equations (LDDE) to capture the non-instantaneous and asynchronous growth of the AHAC for the entire culture time. The delay model was found not only to fit very well the experimental growth curves, but also to confirm the value of some important kinetic parameters. In this study, we are devising a new mathematical model which involves spatio-angular cell-cell interaction coupled with logistic growth. As the cell population evolves, AHAC can change their orientation and position either randomly, or in response to neighboring cells. Experimentally, we observed that when the cells in culture reach a critical level, they spontaneously tend to align along a common axis of orientation. The selection of a preferred axis of orientation stems from the fact that the uniform steady state could be unstable under particular conditions. The model describes the evolution of the cell density in time, space and orientation. The computer simulations require the numerical solution of the integro-partial differential equations that we performed by the moment with a combination of Runge-Kutta method, finite differences and Trapez rule. Our results indicate that we can trust the linear stability analysis, although it cannot predict exactly the behavior of the nonlinear model. In the future, we would like to perform experiments to get some of the parameter values and to check if our mathematical model can predict at least the qualitative behavior of the cells.

Cardiac computations and operator splitting. **Achim Schroll** (Lund universitet, Sweden), Aslak Tveito (Simula Research Laboratory, Norway), Glenn Lines (Simula Research Laboratory, Norway) IC/CT4386/123

During past 10 years [simula.research laboratory] has developed software to simulate the electrical activity of the human heart. Applications of the simulator include: The hearts performance under normal and pathological conditions, predisposing factors for arrhythmias and prospective drug treatments as well as mechanisms of electrical shocks (defibrillation).

Mathematically, the problem is formulated as a system of coupled partial and ordinary differential equations. The ODE system models electro-chemical processes in cardiac cells and recent models tend to be very complicated. This stiff ODE system is nonlinearly coupled to a time dependent reaction-diffusion equation. The complexity of the coupled system makes a straightforward fully implicit approach virtually impossible. That is where operator splitting applies: In an iterative approach the ODE part is step-by-step separated form the PDE part of the model.

The topic of this presentation is to investigate the error of operator splitting applied to the fully coupled discrete model. Under appropriate assumptions, our analysis shows that operator splitting does not reduce the order of convergence of the numerical method. Hence, splitting is an efficient solution technique for the discrete model. Moreover, the ordering of the splitting matters. The error is less if the diffusion step is performed after the reaction step instead of vice versa.

The talk presents joint work with the scientific computing group at Simula, in particular Glenn T. Lines and Aslak Tveito.

The effect of rivers on japanese knotweed *dispersal.* **John Ward** (Loughborough University, UK) IC/CT4498/121

Japanese Knotweed (*Fallopia japonica*) is a highly invasive, rhizomal plant, native to eastern Asia, that has become a major problem in Europe, USA, Canada and New Zealand since their artificial introduction. These plants aggressively displace native species, taking over habitats and reducing biodiversity. Furthermore, their rhizomes (underground stems) are capable of damaging buildings and roads. Management of these plants is made very difficult due to the capability of very small rhizomal fragments to grow and quickly regenerate a knotweed patch. This makes eradication difficult, as the entire rhizome network needs to be removed. Moreover, fragments are easily transported by rivers and canals, which greatly enhances their rate of spread along banks and into new areas.

In this talk, we start by discussing briefly the results of a model of rhizomal spread using a correlated random walks, which motivates the use of Fisher's equation to model events over large time and space scales. These ideas are extended to model the effect river flow on enhancing knotweed expansion both up- and down-stream. By a suitable rescaling, the model reduces to a system consisting of coupled PDEs governing land knotweed density and river fragment density. Travelling wave solutions are investigated in the 1-D case and expansion speeds are determined in terms of the model's parameters with interesting results. Finally, 2-D simulations will be presented to illustrate the impact of river-borne spread.

Geometrical and haemodynamical risk factors for internal carotid artery aneurysm development. **Tiziano Passerini** (Politecnico di Milano, Italy) IC/CT4794/125

The presence of a cerebral aneurysm produces changes in the haemodynamic behaviour of pathological arteries and is related to a non physiological distribution of mechanical stress on the arteries wall. In the context of the ANEURISK project (http://www2.mate.polimi.it:8080/aneurisk) we exploited fluid dynamical analysis of blood flow inside real vascular geometries: these have been reconstructed starting from 3D angiographical images provided by the Department of Neuroradiology of Niguarda Hospital (Milano, Italy). Our goal is to find distinctive morphological and mechanical features related to the risk of development of the pathology.The Navier-Stokes problem in these real vascular geometries is solved numerically with an edge stabilization approach. A realistic (non stationary) flow rate is imposed on the inlet sections through suitable Dirichlet conditions; on the outlet sections we exploit homogeneous Neumann conditions. Different boundary conditions based on the so-called "geometrical multiscale approach" will be addressed too. Post-processing computations lead to the evaluation of dynamical and kinematical quantities such as mechanical stress on the vascular wall and particle trajectories inside the fluid domain.We focus on ICA (internal carotid artery) and find statistical correlations between anatomical and functional features and the presence or absence of aneurysms. A classification of vascular districts is obtained, based on a combination of geometrical (ICA radius, curvature, tortuosity) and fluid-dynamical (wall shear stress, flow vorticity, particle residence time inside aneurysm sac) characteristics. The final goal is to find a risk index, stating the probability of pathology development for arteries belonging to each these classes.

Applications of fuzzy decision making in diabetes. **Venkateshwari Gandhi** (Madurai, India) IC/CT4995/125

Diabetes is a life long disease, thus increasing the morbidity and mortality and decreasing the quality of life. At the same time, the disease and its complications cause a heavy economic burden for the diabetic patients and the society. In this paper, clustering of the diabetic patient is done based on the symptoms such as frequent urination, excessive thirst ,extreme hunger, unusual weight loss, increased fatigue, irritability, blurry vision etc.. The data of the diabetic patient is got from the hospital and from questionnaire. After clustering the patients, fuzzy decision making is considered by which the right remedies can be given to the right patients.

IC/CTS4634/12: Biophysics.

Organiser: Ruediger Ruediger Thul (University of Nottingham, UK)
Co-organiser: Johan Hake (Simula Research Laboratory, Norway)

A bidomain threshold model of intracellular calcium release. **Ruediger Ruediger Thul** (University of Nottingham, UK), Stephen Coombes (University of Nottingham, UK) IC/CT2296/010

We introduce a bidomain threshold model of intracellular calcium release. By the explicit construction of travelling wave solutions we are able to probe the dependence of wave speed on physiologically important parameters, including the rate of calcium pumping between the endoplasmic reticulum and the cytosol. Importantly we develop a linear stability analysis that predicts the onset of front instabilities, leading to the emergence of waves that propagate in a back-and-forth manner. Direct numerical simulations are used to confirm our travelling wave predictions.

Parallel numerical methods for inferring phylogenies. **Nelson Borges** (Instituto Militar de Engenharia, Brazil), Felipe Albrecht (Instituto Militar de Engenharia, Brazil) IC/CT4725/124

In recent years there has been increased interest in producing large and accurate phylogenies trees using some numerical computing approaches. The construction of accurate trees for a large number of taxons requires a computational load increase and thus parallel computing can be helpful[1,2]. We work with distance matrix methods for inferring phylogenies when a large number of taxons is considered. These methods have been introduced by Cavalli-Sforza and Edwards[6] and by Fitch and Margoliash[7] , having given rise to other methods, as those developed by Wolf Y.I. *et al.*[4], Clarke G.D. et al. [3] and Grishin N.V. *et al.*[5]. Cavalli-Sforza methods are associated to a system of linear equations whose dimension grows up linearly with the number of taxons. Here, we use parallel computing to get a lower time processing when solving the associated weakly coupled linear systems. Different iterative methods were performed and compared.

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Stochastic binding of Ca^{2+} *in the dyadic cleft: continuous vs. random-walk description of diffusion.* **Johan Hake** (Simula Research Laboratory, Norway), Glenn Lines (Simula Research Laboratory, Norway) IC/CT3311/122

It is a common understanding that diffusion in signaling micro domains cannot be described properly by a deterministic and continuous model. Several recent publications claim that as the number of participating particles in these volumes goes down, the deterministic description becomes invalid or does not make sense and Random walk (RW) methods have to be employed. We simulate the Ca^{2+} dynamics in a small volume in a myocyte continuously and deterministically by a coupled system of reaction-diffusion equations, and also with a fully stochastic RW model and we stochastically simulate the event of a single Ca^{2+} ions binding to single receptors in both models. The distributions of the bind events from the RW model are used to test the goodness-of-fit of the equivalent distributions predicted by the continuous model, using Kolmogorov-Smirnov tests. We find that the bind distributions from the continuous model fit the collected bind events from the RW simulations. Our results show that if a stochastic model is used for single Ca^{2+} ions binding to receptors in small subcellular volumes, a deterministic and continuous model of the reaction-diffusion dynamics in the actual volume can be used. In our study we also present a novel model for evaluating the stochastic event of a diffusing molecule binding to a stationary or mobile receptor based on a macroscopic rate law. The model is analytical and the accuracy is therefore not dependent on the time step.

The walk of myosin V: a kinetic model. **Rebecca Hoyle** (University of Surrey, UK) IC/CT1312/122

Molecular motors are proteins or protein complexes that transform chemical energy into mechanical work on a molecular level, generating forces and leading to motion. Myosin V is a processive molecular motor involved in intracellular transport that is found in many animal cell types and is particularly plentiful in neurones. It has two heads that attach to an actin track, and a long neck region that attaches to its cargo, such as vesicles and organelles. The coordinated binding and release of the myosin heads to actin result in a walking motion along the track, fuelled by the hydrolysis of ATP.

The precise details of how the biochemical reactions and mechanical motions of the two head elements engineer effective processive molecular motion along actin filaments remain unresolved. In our model (and others) the walk is broken down into substeps and ODEs are given for the time-dependent probability of a myosin molecule being in each of the corresponding substates. We consider five basic states augmented by two others that allow for futile hydrolysis and detachments. We compare the outcomes with experimental results for run lengths, velocities, and dwell times and their dependence on ATP and ADP concentrations and external loads (from attached cargo) in both directions. The model reveals how myosin-V can use the internal strain in the molecule to synchronise the motion of the head elements.

A powerful new feature of our approach is that estimates for the rate constants in the reaction cycle and the internal strain energy are obtained by a computational comparison scheme involving an extensive exploration of a large parameter space. We use simulated annealing to minimise a cost function based on the deviation of our results from experimental data, exploiting the fact that we have obtained analytic results for our reaction network; e.g., for the velocity but also the run length, diffusion constant and fraction of backward steps. The agreement with experiment is often reasonable but some open problems are highlighted, in particular the inability of such a general model to reproduce the reported dependence of run length on ADP concentration. The novel way that we explore parameter space means that any confirmed discrepancies should give new insights into the reaction network model.

Our approach could be used in future to differentiate between competing theoretical models of the myosin-V stepping cycle and indeed between those of other translatory molecular motors, such as kinesins, dyneins and other members of the myosin family.

This work was done in collaboration with Karl I. Skau, formerly of the Department of Mathematics, University of Surrey, UK and Matthew S. Turner of the Department of Physics, University of Warwick, UK.

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Nonlinear dynamics of a double bilipid membrane. **Christine Sample** (Northwestern University, USA), Alexander Golovin (Northwestern University, USA) IC/CT2017/122

The nonlinear dynamics of a double biological membrane that consists of two coupled lipid bilayers, typical of some intracellular organelles such as mitochondria, is studied. A phenomenological free-energy functional is formulated in which the curvatures of the two parts of the double membrane are coupled to the lipid densities. The derived system of coupled nonlinear evolution equations for the double membrane dynamics is studied analytically and numerically. The linear stability analysis is performed and the domain of parameters is found in which the double membrane is stable. For the pa-

rameter values corresponding to an unstable membrane we perform 2-D numerical simulations that reveal various types of complex dynamics.

IC/CTS4641/12: Ecology, epidemiology.

Organiser: Kripasindhu Chaudhuri (Jadavpur University, India)

Mathematical models of fish populations in marine reserves. **Lev Idels** (Malaspina University, Canada) IC/CT4419/121

Marine reserve areas (MRAs) have been proposed as an efficient tool for maintaining a sufficient stock whereas providing a buffer against severe overfishing in the remaining unprotected areas. Based on nonlinear systems of delay differential equations, we build a realistic model of MRAs that incorporates age-structure, migration (dispersal), fishing mortality, variable harvesting rates, and the effects of time delays. In contrast to earlier models, our model is relatively general and may be used to depict a wide variety of circumstances regarding MRAs.

We studied global stability and complex dynamics with perennial ecological favourites such as sign stability, permanence and persistence. The study of the combined effects of periodically varying environment and periodic harvesting rates on the fish population in the reserves will provide practical guidance for specific fishery decisions, e.g., combination of MRAs and seasonal restrictions.

Stability and oscillations of a nutrient–plant–herbivore system with delayed nutrient recycling. **Kalyan Das** (P.P. Poddar Institute, India) IC/CT3614/121

In this paper we consider a mathematical model of a resource Ũbased plant-autotroph-herbivore system with a discrete delayed nutrient recycling and incorporating the average number of herbivores attacking the plants follow the Holling type -II function.we have studied the growth of autotroph and herbivore population depending on the limiting nutrient which is partially recycled through decomposition.It has been shown that the supply rate of external resources play an important role in shaping the dynamics of the autotroph-herbivore system.We have derived the conditions for asymptotic stability and switching to instability of the steady state.The length of the delay preserving the stability has also been derived.Finally,all the analytical results are interpreted ecologically.

Nonlinear models for the effect of pollutants on population with time-delay. **Jamal Hussain** (Mizoram University, Tanhril, India) IC/CT866/121

With rapid pace of industrialization, urbanization, deforestation etc. our environment is getting polluted day by day. The effects of pollution, caused by various human activities on ecosystems have been studied by several researchers. In particular, Parra-Guevara and Skiba (2003) studied the effects of pollutants and control of pollutants emissions. They assumed that a portion of the pollutants emitted to the atmosphere is subjected to various chemical reactions and as a result, a part of a primary pollutant is transformed into other substances (secondary pollutants), which can be more toxic than the original one. But in the above studies the effect of time lag has not been considered. In this regard, Rescigno (1977) studied the effect of precursor pollutant on single species, but he did not consider the rate of uptake concentration of the pollutant on the growth of the species. Further in the above studies the effect of diffusion has not been considered. Keeping the above in view, in this paper we propose and analyse the effect of a pollutant on a population, which is living in an environment polluted by its own activities. It has been assumed that the pollutant enters into the environment not directly by the population but by a precursor produced by the population itself. It has been further assumed that the larger the population, the faster the precursor is produced, and the larger the precursor, the faster the pollutant is produced. The model has been studied with and without diffusion. In the case of no diffusion it has been shown that population density settles down to its equilibrium level, the magnitude of which depends upon the equilibrium levels of the emission and washout rates of pollutant as well as on the rate of precursor formation and its depletion. It has been noted that the rate of precursor formation is crucial in effecting the population. It has further been noted that if the concentration of pollutant increases unabatedly, the survival of the population would be threatened.

The effect of diffusion on the interior equilibrium state of the system has also been investigated. It has been shown that if the positive equilibrium of the system without diffusion is globally asymptotically stable, then the corresponding uniform steady state of the system with diffusion is also globally asymptotically stable. It has further been noted that if the positive equilibrium of the system with no diffusion is unstable, then the corresponding uniform steady state of the system with diffusion can be made stable by increasing diffusion coefficients appropriately. Thus, it has been concluded that the global stability is more plausible in the case of diffusion than the case of no diffusion.

In case of conservation model, it has been shown that if the rate of formation of the precursor pollutant is controlled by some external means, its effect on the population can be minimised.

Numerical Simulations are also carried out to validate the models developed.

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Biological control through provision of additional food to predators: a theoretical study. **Srinivasu Pichika** (Andhra University, India), Prasad Bhuvanagiri (Andhra University, India), Venkatesulu Mandadi (University of Missouri, USA) IC/CT975/121

In this article we analyze a variation of a standard predator-prey model with type II functional response which represents the predator-prey dynamics in presence of some additional food to the predator. The aim is to study the consequences of providing additional food on the system dynamics. We conclude that handling times for the available foods play a key role in determining the eventual state of the ecosystem. It is interesting to observe that by varying the quality and quantity of additional food we can, not only control and limit the prey but also limit and eradicate the predators. In the context of biological pest control, the results caution the manager on the choice of quality and quantity of the additional food used for this purpose. An arbitrary choice may have opposite effects leading to increase in pest concentration and eradication of the predator. From this study it is possible to develop management strategies that manipulate quality of the additional food and its supply level for the benefit of biological control. The theoretical conclusions agree with results of some practical biological control experiments.

Mathematical modelling on harmful algal blooms in the presence of toxic substances. **Samares Pal** (RKM Vivekananda Centenary College, India) IC/CT730/121

Plankton is the basis of the entire aquatic food chain. Phytoplankton, in particular, occupies the first trophic level. Plankton performs services for the Earth: it serves as food for marine life, gives off oxygen and also absorbs half of the carbon dioxide from the Earth's atmosphere. The dynamics of a rapid (or massive) increase of plankton populations is an important subject in marine plankton ecology and generally termed as a 'bloomŠ. There has been global increase in harmful plankton in last two decades and considerable scientific attention towards harmful plankton has been paid in recent years.

The model that we propose has three interacting components consisting of the non-toxic phytoplankton (NTP), herbivorous zooplankton (Z) and toxin producing phytoplankton (TPP) with an additional factor that the release of toxic substance by toxic-phytoplankton species reduces the growth of zooplankton.

To establish the theoretical results we shall use our field observations. We consider the toxin producing plankton (TPP) species as Noctiluca scintillans, non-toxic phytoplankton (NTP) species as Coscinodiscus sp. and zooplankton species as Paracalanus sp. Our field study suggests that when TPP is absent the equilibrium level of NTP is much lower than the value observed when TPP is present. Moreover the equilibrium level of zooplankton decreases when TPP is present. This phenomenon depicts the fact that the presence of TPP in the system enhances the production of NTP and reduces the zooplankton grazing pressure. Further, the biomass distribution observed in our field study demonstrate that introduction of TPP leads to the persistence of all the species through reduction of blooms and can be used as controlling agent for stability of marine ecosystem. Our analytical as well as numerical study reveals the essential mathematical features regarding the role of TPP in phytoplankton-zooplankton interaction.

On selective harvesting of an inshore–offshore fishery: a bioeconomic model. **Kripasindhu Chaudhuri** (Jadavpur University, India) IC/CT456/121

In the present paper, a bioeconomic model is developed on the selective harvesting of a single species inshore-offshore fishery, assuming that the growth of the species is governed by the Gompertz law. Our motivation for introducing the Gompertz law primarily lies in the superiority of the Gompertz law over the logistic law. Since ideal living conditions prevail in the initial stage, there should be very rapid growth initially. Thereafter, as the population grows, the limitation of resources forces the growth rate to decline and the population gradually approaches the saturation level. Compared to the logistic law, the Gompertz law exhibits faster early growth, but a slower approach to the asymptote, with a longer period of linear growth about the point of inflexion.

When the fish population size becomes considerably large, it tends to maintain a strong pressure on the newly produced biomass through cannibalism which is more effective on larger egg-aggregates formed by overcrowding of eggs in a large fish population. Also, there will be intraspecific competition amongst the individuals in the population for the use of limited resources available in the habitat. These effects, coupled together, should retard the growth of the population to a large extent and as a result, the population size should approach its asymptote rapidly as in the case of the logistic model. These retarding effects are, however, counterbalanced to some extent by group movement which is a special behavioural characteristic of a fish population. As a result, the approach of the population size to the asymptote is slowed down. This peculiar feature of faster early growth and slower approach to the asymptote is reflected in the Gompertz law of growth. Moreover, implications of exploiting a biological population obeying the Gompertz law of growth have been studied very little. This fact also motivated the author to develop the present model.

The dynamical system governing the fishery is studied in depth. The local as well as global stability of its non-trivial steady state is examined. Existence of a bionomic equilibrium is established under different parametric considerations. The optimal harvest policy is discussed by invoking PontryaginŠs Maximal Principle. Lastly, the results are illustrated with the help of a numerical example.

IC/CTS4636/12: Tumor and cardiac modelling.

Organiser: Graeme Wake (Massey University, New Zealand)

Multiscale modelling of fluid transport in tumours. **Rebecca Carter** (University of Oxford, UK), Jon Chapman (University of Oxford, UK) IC/CT4280/123

The success of therapeutic agents in treating cancer is limited by their inability to reach their target *in vivo* in adequate quantities. Rapid cell proliferation rates and a lack of functioning lymphatics in tumours result in a poorly organised vasculature and an increased interstitial fluid pressure, limiting delivery of drugs to malignant cells and causing the development of hypoxic (oxygen deprived) and necrotic regions. To fully exploit anticancer drugs it is crucial to understand and overcome the physiological *barriers* to their penetration.

With this in mind, we aim to develop a comprehensive mathematical model for the transport of blood through a tumour. We assume the tumor has a periodic microstructure and consider a *unit cell* made up of blood vessels and surrounding tissue. Blood is treated as a Newtonian fluid and the high permeability of tumour capillary walls is captured using Starling's Law to model the extravasation of fluid from the capillary into the interstitium. We solve the flow problem on this local scale and use multiple scales to drive the effective equations describing the blood transport on the tumour scale. Similarly we incorporate convection and diffusive drug transport to give effective equations that describe the distribution of the drug throughout the tumour.

Modeling the migration of cancer cells in the bloodstream. **Keng Hwee Chiam** (IHPC, Singapore) IC/CT1144/122

We model the migration of cancer cells that have broken away from a tumor and are circulating in the bloodstream. Using the immersed boundary method and culling from literature the material properties of cancer cells, we simulate how cells deform as a function of the flow properties of the bloodstream as well as the adhesive properties between the cancer cells and the endothelial cells of the bloodstream. We also simulate the migration characteristics as a function of the migrating cell density. From these, we calculate rough approximations of the metastatic rate and efficiency. Finally, we speculate on how our discrete cell modeling approach can be connected to continuous modeling approaches of tumor growth.

Functional differential equations arising in cell-growth models. **Graeme Wake** (Massey University, New Zealand) IC/CT4810/123

In the course of developing generic models of the evolution of cell cohorts simultaneously undergoing growth and fission, which are structured by size (here taken as DNA content), we have encountered an unusual class of functional differential equations. The solution of these possess the behavior described as a "steady-size distribution(SSD)", where the size distribution is constant in shape, but not magnitude, as time evolves. These equations do not fit easily into established theory as there is a distinct lack of general theory of non-local differential equations. Yet the non-local character is exactly what determines the occurrence, asymptotically with time, of SSD-like behavior. These equations are shown to have solutions which are candidates for probability distributions by a range of techniques. This means identifying the eigenvalues of a singular, non-local, eigenvalue problem. The SSD-like behavior is usually globally attracting, but this is not yet established in general. These models describe actual cell-population cohorts and the match with data of tumor cells (in-vitro data) is excellent. The model can be changed to describe the cohort evolution under tumor treatment and to assess the effectivenes of cancer therapy. The latter, by switching off the non-local term in the equations, destroys the SSD-like behaviour. This work is being extended to models incorporating non-linear growth effects. Work done in collaboration with Ronald Begg and Bruce van-Brunt (Massey University), Bruce Baguley and Elaine Marshall (University of Auckland), and Britta Basse and David Wall (University of Canterbury). The support of the NZ Institute of Mathematics and its Applications by the award of a Maclaurin Fellowship during the current part of this work is gratefully acknowledged.

Thin-film modelling of bacterial swarming. **Eleanor Norris** (Loughborough University, UK), John Ward (Loughborough University, UK) IC/CT4505/010

Swarming is a term used to describe the rapid spread of bacterial colonies on a moist semi-solid substrate. The phenomenon is cell density dependent and usually occurs in response to low nutrient levels. Swarming plays an important part in many bacterial infections, including wound infections and septicaemia as well as lung infections in, for example, cystic fibrosis patients. We aim to develop an understanding of the processes involved in bacterial swarming with the eventual aim of using this knowledge to compare different treatment strategies. Our work involves developing a model of swarming bacteria constrained within a thin film. The equations describing the biological mechanisms determining the behaviour of the bacteria are coupled with the standard thin-film reduction of the Navier-Stokes equation (which describes the action of the biosurfactant on the fluid boundary). The initial results of this modelling will be presented, along with a comparison of these results with the available experimental data.

IC/CTS4642/12: Other medical applications.

Organiser: Martin Frank (TU Kaiserslautern, Germany)

Clustering the individuals using similarity measure by their life style. **Kameshwari Meenakshi Sundaram** (Thiagarajar College of Engineering, India), Venkateshwari Gandhi (Madurai, India), Velu Lakshmana Gomathi Nayagam (NIT Tiruchirappalli, India) IC/CT3890/125

Diseases caused by the life style are becoming a huge burden to the society. To cure these diseases, the study about the life style of the individual is needed. The patients affected by the same life style may need same remedies. The life style of them has been studied by the questionnarie. Questionnarie contains the criterias such as workload, familial background etc. The information from the individuals would be in Intuitionistic Fuzzy linguistic terms such as high, low, normal, fair , good etc. Those Intuitionistic Fuzzy linguistic terms are converted to Intuitionistic Fuzzy Number using the dilation and concentration properties of Intuitionistic Fuzzy set by fixing one of the linguistic terms as F. Similarity measure has been found out by using the Euclidean distance measure. By defining equivalence relation the individuals are clustered. A medical practitioner can then counsel or give remedies to these clustered individuals.

Keywords: Intuitionistic Fuzzy Set, Similarity measure , Euclidean distance in Intuitionistic Fuzzy setup, Intuitionistic Fuzzy Number,Dilation ,Concentration.

Travelling-wave behaviour in a multiphase model of a population of cells in an artificial scaffold. **Greg Lemon** (University of Nottingham, UK) IC/CT4763/125

In this talk I will discuss travelling-wave behaviour in a recently-formulated multiphase model for the growth of biological tissue in the context of tissue engineering. In suitable limits, tissue growth in the model is shown to occur in the form of travelling waves that can propagate either forwards or backwards, depending on the values of the parameters. In the case where the drag force between the cells and the scaffold is non-zero, the growth can be analysed in terms of the propagation of a constant-speed wavefront in a semi-infinite domain. A shooting method is described for numerically calculating the wave speed, and results for how the speed varies with respect to the parameters are given. In the case where the drag force is zero, the size of the aggregate of cells is shown either to grow or to shrink exponentially with time. I will also give some asymptotic results of the convergence to the travelling wave solutions. The results presented in this talk may be of importance in determining the experimental factors that control tissue invasiveness in scaffolds thereby allowing greater control over engineered tissue growth.

Work done in collaboration with Professor John King.

Toward fast and accurate deterministic models for dose calculation in radiotherapy. **Martin Frank** (TU Kaiserslautern, Germany) IC/CT1008/125

A deterministic Boltzmann transport model for dose calculation in electron radiotherapy is presented. We investigate several ways to simplify the deterministic model having two goals in mind: lower computation times on the one hand, high accuracy and model inherent incorporation of tissue inhomogeneities on the other hand. While being fast, the second property is lost in the often used pencil beam models. Several test cases, including the irradiation of a water phantom, are presented.

Identification of muscle determinant for different gait speeds by proper orthogonal decomposition. **Sirod Sirisup** (National Electronics and Computer Technology Center, Thailand), Rumpa Boonsinsukh (Srinakharinwirot university, Thailand) IC/CT1108/015

In this investigation, we explore the use of the proper orthogonal decomposition (POD) on electromyography (EMG) of the leg muscles, with the objective of elucidating the musclesŠ behavior for each gait speeds. Four different gait speeds were used in the study: slow, comfortable, faster and fastest walking. The electromyographic data used in this study were recorded from 12 bilateral lower limb muscles: tensor fascia latae (TFL), semitndinosus (ST), vastus medialis (VM), rectus femoris (RF), tibialis anterior (TA) and medial gastrocnemius (MG). Results indicate that the primary muscles for slow walking were bilateral TFL which act alternately to accept weight bearing on each leg. The same muscles also show another dominant function when working simultaneously in pelvic stabilization. In addition, we found that when the speed of walking increases, the number of muscle determinants for gait has been added. This study emphasizes that the POD method is the novel method to identify the energy-efficient gait such that comfortable walking is the most energy-efficient gait, whereas fastest walking consumes the highest energy.

A drug–drug interaction parameter-estimation problem, II. **Bruno Bieth** (Purdue University, USA), Raymond Chin (Indiana University & Purdue University, USA), Lang Li (Indiana University, USA) IC/CT779/125

A two drug interaction is usually predicted by individual drug pharmacokinetic. An innovative drug-drug interaction prediction method based on a three-level hierarchical Bayesian meta-analysis model is developed that includes a Monte Carlo Markov chain pharmacokinetic parameter estimation procedure. Underlying the parameter estimation procedure is a fast integration method of the stiff pharmacokinetic equations. In this presentation, we report the results of the fast integration method on the system of stiff pharmacokinetic equations. We also discuss the interrelation and interaction between the Monte Carlo Markov chain pharmacokinetic parameter estimation procedure and the numerical integration scheme.

12: Bio-Mathematics, Posters

IC/PP4390/012: **Theoretical vs. experimental analysis of neurogenesis models.**

Presenter: Yanthe Pearson (Rensselaer Polytechnic Institute, USA)

Normally, the growth of neuronal processes is highly regulated, with temporally-controlled initial outgrowth followed by regular cycling between phases of extension and retraction as the processes navigate toward their targets. Ethanol delays the initial outgrowth of axons and dendrites, but the dynamics of subsequent growth are altered in rather specific ways. We apply stochastic techniques through mathematical modelling of this biological process with an emphasis on the axons spatial behaviour, under certain conditions. Current experimental studies use time-lapse microscopy of live embryonic rat hippocampal neurons, growing in cell culture, to study the dynamics of axonal and dendritic growth and the consequences of the disruption of their growth, by the use of ethanol. We choose to explore such phenomenon for several reasons, those of which include assisting biologists in providing them with approximations through sophisticated quantitative analysis of their experiments, as well as a means to explore methods for future studies, biological and/or other disciplines. Our approach includes careful analysis of data, by various methods, those of which include filtering, inverse techniques, Markov chain methods, as well as noise reduction and time series analysis. We then introduce simple stochastic models, based on variables defining the axons movement; these models are studied both numerically and analytically, as a means to capture the phenomenology underlying the axons internal and external mechanisms, as well as to acquire and compare parameter estimates.

IC/PP4790/010: **Coupled calcium and cell-cycle dynamics in radial glial cells.**

Presenter: Duncan Barrack (University of Nottingham, UK)

Radial glial cells give rise to neurons via asymmetric division during the embryonic development of the brain and communicate via ATP mediated calcium waves, with ATP being released into the extracellular space as the cell approaches S phase of the cell cycle. ATP then binds to the $\mathrm{P2Y_1}$ receptors of radial glial cells, leading via a G-protein cascade to the release of calcium from internal stores. Internal calcium transients have the effect of increasing the production of Cyclin D, a key regulator of cell cycle progression. This coupling is thought to locally synchronise cell cycles, so that clusters of cells proliferate together, shedding cells in uniform sheets.

There are various models for the cell cycle and for intracellular calcium dynamics. We present a model that couples the calcium and cell cycle dynamics in a radial glial cell. We then use a combination of direct simulation and numerical continuation of periodic solutions to study the effect of this coupling on the period of the cell cycle. When cells in a 1D lattice communicate via the diffusion of extra-cellular ATP, a phase averaging technique shows that this spatial coupling can lead to the phase locking of the cell cycles. We consider how this synchronous behaviour depends upon different parameter regimes. For example, we consider a regime where cells are intrinsically cycling, as well as regimes where cells are quiescent (i.e., not cycling) until an initiating ATP pulse leads to the release of calcium in that cell, inducing it to enter the cell cycle and leading to a propagating calcium wave with concomitant effects on the cell cycle throughout the lattice of cells. We also look at how stochastic calcium events affect the local synchronisation of the cell cycle.

IC/PP1685/010: **Gene-regulatory networks and delay-differential equations.**

Presenter: Arcady Ponosov (Universitetet for Miljø- og Biovitenskap UMB, Norway)

A mathematical framework to study gene regulatory networks with time-delay effects, which is based on delay differential equations, is suggested and outlined. An essential feature of the gene regulatory networks is their “almost Boolean” structure, where the dynamics are governed by sigmoid-type nonlinearities which are close to the step functions. This is due to the fact that genes are only activated if certain concentrations are close to the respective threshold values. The delay effects arise from the time required to complete transcription, translation and diffusion to the place of action of a protein. Compared to biomolecular reactions with a typical time scale of seconds or fractions of a second, these processes are slow: it may take several minutes or even hours from the binding of the transcription factor to the promoter until the transcription

and translation process is finished.

Any mathematical model describing such networks faces a problem of how to study the dynamics in the vicinity of the thresholds. A method of localizing stationary points and local stability analysis near the thresholds in the presence of delays is offered. The basic technical tools, which are systematically applied within the suggested framework, combine a special modification of the well-known “linear chain trick" with the perturbation analysis.

Some properties of gene regulatory networks with delay in comparison with the non-delay model are discussed as well.

The results are illustrated by a number of examples.

Acknowledgment. The work is partially supported by CIGENE - Centre for Integrative Genetics at the Norwegian University of Life Sciences.

IC/PP4711/015: Modelling planar cell polarity.

Presenter: Sabine Schamberg (University of Nottingham, UK)

Planar Cell Polarity (PCP), the phenomenon of whole fields of cells being polarised in a plane, is a common feature in insects and mammals. Typical examples are the alignments of scales, hairs, feathers or bristles. The animal most studied in this context is the fruit fly *Drosophila*. In this work we concentrate on its wings in which every cell elaborates a hair that points distally. Although the mechanism of PCP is still not completely understood, the core proteins have been found and some theoretical studies have been conducted. Since a lot of biological details are included into these models they tend to be rather complex and therefore difficult to analyse mathematically. Hence our aim is the development of alternative simplified models and the simplification of already existing ones, which facilitates their analysis. In this work, we present two such approaches.

The first one is a simplified model in one spatial dimension. Here, we consider a row of cells, whereby each cell has two sides with a certain amount of activity (corresponding to accumulation of certain PCP proteins) on each side. The activity in a cell is then moved back and forth in that cell depending on the amount of activity in the neighbouring cells. The more activity there is on the adjacent side of the next cell, the more is moved away from the present side to the other one within the same cell. In addition the amount that is moved depends on the level of concentration on the present side. This mechanism results in polarisation of the cells, which in certain cases is even propagated as a wave. The speed of this wave depends on the rate of impact of the neighbouring cells on the present cell. This approach can be extended to arrays of square or hexagonal cells in two spatial dimensions.

Furthermore we analyse the model proposed by Amonlirdviman *et al.* (*Science, 307:423-426, 2005*). This consists of a system of reaction-diffusion equations, which describe the interactions of the core proteins in a field of two-dimensional hexagonal shaped cells. The polarisation is driven by two main mechanisms: a negative feedback loop and an intrinsic spatial bias. In order to perform a numerical steady state analysis of this approach we have simply considered the one space dimensional case and assumed that, similar to the simplified model discussed above, we have a row of cells in which each cell has two sides, a left and a right one. These investigations revealed that PCP can be achieved without the intrinsic bias, provided there is an initial intracellular inhomogeneity which can be amplified.

IC/PP7/121: Effect of age-based vaccination policy on the dynamics of delay epidemic model.

Presenter: Sumit Banerjee (JSS Academy Of Technical Education, India)

The spread of communicable diseases depend on rate of transmission or contact rate, removal rate, mode of transmission , latent and incubation period, age Ű specific susceptibility and immunity of individuals to the disease . The immunity to the specific disease in the individuals can be artificially developed with the help of vaccination. It is understood that the vaccination leads to complete protection and vaccinated individuals are immune but this is not true and in general vaccination only leads to partial protection. The role of latent period in the dynamics of communicable diseases is also an important factor and should be considered in the epidemic models. Further, while studying age-structured epidemic models, maturation period should also be considered in the model, because in the case of several infectious diseases the populations of certain Age Ű groups are immune from diseases for some finite period and after that they become susceptible.

In view of the above, therefore, in this paper a delay epidemic model has been studied to investigate the effect of age Ű based vaccination policy on the dynamics of a communicable disease incorporating latent period and maturation delay. For the model, the disease-free and endemic equilibrium points have been obtained and their local and global stability analysis have been carried out .

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IC/PP4354/121: Parasitoids may act as bodyguard for maize plant by attacking pests: a mathematical model.

Presenter: Guruprasad Samanta (Department of Mathematics, Bengal Engineering and, India)
Co-author: Alakes Maiti (Presidency College, Kolkata, India)

Maize (*Zea mays*) is an important food crop world-wide and *Spodoptera* sp. (e.g., fall armyworm *Spodoptera frugiperda*) are important pests of this. The farmers have to suffer from heavy economic losses due to these pests. In this paper, we have examined the usefulness of natural enemies from the viewpoint of the plant fitness. We have considered a tritrophic model consisting of maize plant, pest and parasitoid to analyze the field observations. The effect of time-delay on the tritrophic model is studied. Numerical simulations are carried out to illustrate our mathematical findings. The implications of our results are discussed critically.

IC/PP2016/122: Modelling macromolecular transport in the interphase cell nucleus.

Presenter: Annika Wedemeier (German Cancer Research Center, Germany)
Co-author: Joerg Langowski (German Cancer Research Center, Germany)
Co-author: Willi Jaeger (Universität Heidelberg, Germany)
Co-author: Holger Merlitz (Xiamen University, PR China)
Co-author: Mario Mommer (Interdisziplinäres Zentrum für wissenschaftliches, Germany)

In recent years great progress has been made in the view of the living cell as a regulatory network in time. However, a quantitative description of the transport of biomolecules in the dense macromolecular network of chromatin fibers in the interphase cell nucleus is still missing. Furthermore, it is not yet clear to what extent macromolecular mobility is affected by structural components of the nucleus.

This work contributes to the understanding of this process by developing a theoretical description of network diffusion in the interphase cell nucleus. To model the situation in the cell nucleus a lattice approach is used minimizing computational time and effort. Our model leads to a quantitative understanding of transport behaviour which is directly related to chromatin morphology. Changes of these characteristics are known to occur upon apoptosis or malignant transformations.

The crowded environment of chromatin fibers in the nucleus is simulated by a simplified version of the bond fluctuation method originally desrcibed by Carmesin et al (Macromolecules 1988,21, p.2819) in combination with a Metropolis Monte Carlo procedure. This yields well equilibrated polymer chains satisfying static properties such as end-to-end distance.

It is investigated how the diffusion coefficient of particles of a given size depends on the 3D geometry of the network of chromatin fibers and their density in the nucleus. We show that the diffusion cofficient is proportional to the volume fraction of the freely accessible space. Additionally, we investigate to what extent structural properties of the fibers, such as persistence length and contour length, influence the diffusion coefficient. We observe that neither the contour length nor the persistence length of the fibers affects the diffusional transport of small particles.

Furthermore, we found that the translational diffusion of the mass centers of the chromatin fibers is anomalous.

The concentration of the biomolecules in the cell nucleus over time is predicted by an analytical reaction-diffusion model. The diffusion coefficients of this system are fitted to the results obtained by the numerical lattice approach.

IC/PP4760/123: Finite-element analysis for radio-frequency ablation of infarcted cardiac tissue.

Presenter: Jacques Beaumont (Binghamton University, USA)
Co-author: Ying Sun (Binghamton University, USA)
Co-author: Fan Zhou (SUNY Binghamton, USA)

Radiofrequency (RF) ablation is the treatment of choice for cardiac arrhythmias occurring in myocardial infarction. While preferred over drug treatment, RF ablation presents a number of risks, especially microexplosions and severe bleeding due to excessive heating. Our goal is to optimize the parameters of RF ablation in order to produce a minimal amount of damage while still preventing the formation of micro-reentrant circuits within the infarcted zone. To this end, we have developed a finite element (FE) model of myocardial infarcts and RF induced tissue damages. The model provides means by which noninvasive cardiac imaging data can be used to determine optimal parameters of RF ablation. Our thermo-electric coupled FE model has two innovative elements. First, it takes into consideration both perfused and non-perfused tissue (multizone) encountered in an infarcted area and how RF changes this distribution in time. Second, it incorporates a realistic geometry of the infarct including isthmuses by which impulses can reenter. Solving the thermo-electric coupled problem, we determine the lesion size during ablation. A RF stimulation with a power of 10W-35W is investigated for various penetration depths, infarct geometries, blood perfusion rates, and operation periods. We found that the blood perfusion can significantly reduce the maximum tissue temperature and lesion size, and hence lower the possibility of microexplosions and blood coagulation. The lesion grows rapidly at the very beginning of the operation and slows down as it reaches quasi-steady state. The results indicate that a 20W stimulation of 100s can produce a lesion large enough to prevent most micro-reentrant circuits located near the surface. However, blocking conducting pathways deep inside the infarct may need extra power input. With appropriate experimental validations, we plan to utilize our model to determine optimal parameters for RF ablation, and investigate artificial perfusion needed for interventions.

IC/PP3179/015: Instabilities in biochemical reaction networks.

Presenter: Maya Mincheva (University of Wisconsin, USA)

Understanding interactions in complex biochemical reaction networks of genes, proteins and enzymes is an important problem in modern cellular biology. Mathematical models of biochemical reaction networks are usually large systems of coupled nonlinear differential equations with many unknown parameters, making direct numerical simulations practically impossible.

On the other hand, important properties of these systems are determined only by the network's structure, and do not depend on the unknown parameters. We describe how a bipartite graph associated with a biochemical reaction network can be used to predict its dynamical properties, such as multistability and oscillations, usually referred to as instabilities. This analysis generalizes the positive/negative feedback cycle conditions for instabilities.

In more general models, the instabilities can be caused by diffusion or delays. Similar network conditions relate the structure of the same bipartite graph to delay-induced or diffusion-driven phenomena, such as oscillations or Turing instability respectively.

The proposed method is suitable for computerization, which will enable the analysis of large biochemical networks with incomplete kinetic data.

13: Physics and Electrical Engineering, Minisymposia

IC/MP3896/010: **Path integrals, classical waves, quantum waves, and modern mathematical asymptotics, II: coherent state representations, novel mathematical extensions, and computational, seismic, and electromagnetic applications.**

Organiser: Bair Budaev (University of California, Berkeley, USA)
Co-organiser: Louis Fishman (MDF International, USA)

Ever since Feynman's ground breaking path integral formulation of quantum mechanics in the 1940's, path integrals have played an increasingly important role in quantum field theory, condensed matter physics, mathematics, and classical physics and engineering applications. This minisymposium will examine path integrals and their applications from the perspective of the correspondence between classical wave propagation, quantum mechanical wave propagation, and the development of modern mathematical asymptotics. Coherent state constructions will be discussed. Novel mathematical extensions will be presented. A Feynman–Kac-type stochastic formulation for the Helmholtz equation will be developed and applied in electromagnetic modeling. Applications to seismic wave propagation and imaging, and electromagnetic modeling will be discussed. The design of a specific computing architecture for the rapid evaluation of path integrals will also be addressed.

Envisioning light: software-assisted research in optical singularities. **Michael Berry** (University of Bristol, UK) IC/MT1098/011

Singularities of fields of light rays and waves of light are increasingly recognized as fundamental in optics. In exploring these singularities, mathematical software has played a central role, in computation and in visualizations that have led to the discovery of new phenomena.

At the geometrical level, the singularities are caustics— surfaces on which focusing occurs. Waves decorate these with rich interference patterns, whose finest structures are new singularities, namely singularities of phase (a.k.a. nodal lines, or optical vortices, or wave dislocations). The vector nature of light introduces further singularities, associated with polarization.

Many phenomena are best understood and illustrated in terms of singularities: rainbows, tsunamis, polarization fingerprints in the blue sky, the complexities of crystal opticsĚ

Wiener-measure regularized path-integrals: the right mathematics, the right physics. **John Klauder** (University of Florida, USA) IC/MT959/010

Feynman's formal phase-space path integral lacks physical as well as mathematical meaning. Insertion of a regularizing factor leading to a Wiener measure on phase space, coupled with a limit outside the integral in which the diffusion constant diverges, gives the integral both mathematical and physical meaning. For diffusion on a plane (or a sphere, or a pseudosphere), the result is a propagator expressed in a coherent-state representation appropriate to canonical (or spin, or affine) kinematics. Adoption of the Stratonovich midpoint rule leads to a well-defined path integral that is covariant under canonical coordinate transformations. With a well-defined path integral in hand, suitable semiclassical asymptotics may be developed.

A multi-scale approach to one-way wave propagation. **Maarten de Hoop** (Purdue University, USA) IC/MT3695/010

Starting from a Trotter product representation, we develop a multi-scale approach to one-way wave propagation derived from dyadic parabolic decomposition in phase space. The associated thin-slab propagator is related to a pseudodifferential operator. We obtain an expansion of the thin-slab propagator revealing a separation of variables in phase space reminiscent of the generalized-screen expansion. We discuss various numerical aspects.

Joint research with H. Smith (UW), G. Uhlmann (UW), F. Andersson (Lund).

Numerical implementation of seismic wavefield operators via path integrals. **Michael Lamoureux** (University of Calgary, Canada), Gary Margrave (University of Calgary, Canada) IC/MT2915/010

The seismic imaging problem centers around mathematical and numerical techniques to create an accurate image of the earth's subsurface, using recorded data from geophones that capture reflected seismic waves. Using a path integral approach, a wavefield extrapolater can be expressed as a limit of depth-sliced path steps through a variable velocity medium. An image is created from the correlation between upward and downward going waves. We report on the mathematical issues that arise in implementing numerical algorithms based on the path integral approach, in particular convergence, stability, and accuracy.

IC/MP160/010: **Path integrals: classical waves, quantum waves, and modern mathematical asymptotics, I: phase-space constructions, convergence issues, and seismic and electromagnetic applications.**

Organiser: Bair Budaev (University of California, Berkeley, USA)
Co-organiser: Louis Fishman (MDF International, USA)

Ever since Feynman's ground breaking path integral formulation of quantum mechanics in the 1940s, path integrals have played an increasingly important role in quantum field theory, condensed matter physics, mathematics, and classical physics and engineering applications. This minisymposium will examine path integrals and their applications from the perspective of the correspondence between classical wave propagation, quantum mechanical wave propagation, and the development of modern mathematical asymptotics. Phase space constructions will be discussed, and their connections to wave propagation and inverse scattering algorithms displayed in detail, for both the cases of one- and two-way wave equation modeling. The role of path integrals in electromagnetic modeling will be reviewed. Mathematical convergence issues will be discussed, along with a presentation of applications to seismic wave propagation and imaging.

Probabilistic approach to wave propagation. **Bair Budaev** (University of California, Berkeley, USA), David Bogy (UC Berkeley, USA) IC/MT2063/010

The similarity between the Helmholtz and Schrödinger equations creates opportunities for extending the ideas conceived in quantum mechanics to wave propagation and vice versa. Thus, ray theory of wave propagation brought transparent asymptotic solutions to some problems of quantum physics, while path integrals associated with the Schrödinger equation provided theoretically exact solutions to problems of wave propagation which lead to an insightful alternative view of ray theory. The advantages of such cross-fertilization become especially valuable when methods originating from different areas are combined to compensate the deficiencies of each method by the strengths of the counterparts.

Here we discuss a novel approach to wave propagation which combines the ideas of ray theory with the technique of path integration. This approach starts similarly to ray theory, from the representation of the solution of the Helmholtz equation as a product of the amplitude and the oscillating exponent of the eikonal, which is computed by a canonic technique of analytic mechanics. However, unlike in ray theory, the amplitude is not approximated by the exact solution of the approximate first-order transport equation, but instead, the amplitude is considered as the solution of the complete transport equation which is exactly equivalent to the original Helmholtz equation. Then the complete transport equation is solved by the probabilistic Feynman-Kac formula based on the path integral with respect to the Wiener stochastic measure associated with the heat-conduction equation, which is much better suited for computations than the path integral associated with Schrödinger equation.

This approach to wave propagation is shown to be an effective tool for the analysis of numerous wave propagation problems some of which are notoriously difficult for standard methods, and the proximity between the Helmholtz and Schrödinger equations makes it natural to expect that the advantages of the method are not restricted to wave theory, but will also find useful application to quantum mechanics.

Path integrals as analysis on path space by time-slicing approximation. **Naoto Kumano-go** (Kogakuin University, Japan) IC/MT1640/010

In 1948, R.P. Feynman expressed the integral kernel of the fundamental solution for the Schrödinger equation, using the path integral. The path integral is a new sum over all paths. Feynman explained the path integral as a limit of the finite dimensional integral which is now called the time slicing approximation. Furthermore, Feynman suggested a new analysis on a path space with the functional integration and the functional differentiation. However, in 1960, R. H. Cameron proved that the measure of the path integral does not exist mathematically. Therefore, using the time slicing approximation, we treat the path integral as an analysis on a path space by a mathematically rigorous discussion.

Samplers for the Feynman–Kac or Onsager–Machlup formulas. **Cristian Predescu** (University of California, Berkeley, USA) IC/MT4165/130

In chemical physics, the Feynman–Kac formula is utilized to evaluate quantum effects by path integral Monte Carlo simulations. The Onsager-Machlup formula provides the sampling distribution for a Smoluchowski process, albeit the Feynman-Kac formula can be utilized to the same effect. In both cases, there is there need for Monte Carlo samplers capable of coping with the critical slowdown that appears when the number of path variables becomes large because of accuracy requirements or large transit times. I shall present the fast sampling algorithm and the sliding and sampling procedure, which are capable of addressing these issues to various degrees.

Helmholtz path integrals. **Chad Hogan** (University of Calgary, Canada), Louis Fishman (MDF International, USA) IC/MT4984/130

The multi-dimensional, scalar Helmholtz equation plays a prominent role in modeling both classical (acoustics, electromagnetics, optics, seismics) and quantum mechanical wave propagation phenomena. In 1948, Feynman introduced the path integral representation for the fundamental solution of the (one-way) Schrödinger equation of non-relativistic quantum mechanics. These coordinate and phase space, functional integral solutions provide a convenient global statement of the wave propagation process, identify important physical quantities, connect to an underlying stochastic foundation, and naturally lead to computational algorithms. Corresponding path integral constructions for the Helmholtz equation are complicated by the inherently two-way nature of this *elliptic wave propagation* problem.

This talk will briefly review several different approaches to the construction of Helmholtz path integrals. After a concise review of the Feynman path integral constructions for the Schrödinger equation, the Feynman/Fradkin representation, based on the imbedding of the n-dimensional Helmholtz equation in an $(n+1)$-dimensional Schrödinger equation, will be examined. This will lead naturally to the approximate Feynman/Garrod path integral representation for the Helmholtz equation. The application of the Liouville representation and the Feynman-Kac formula will then follow. Changing direction, the exact, well-posed, one-way reformulation of two-way, elliptic wave propagation problems, based on the Dirichlet-to-Neumann operator and corresponding phase space path integral constructions, will be reviewed. Subsequently, these solution representations will be contrasted with the corresponding coordinate space path integral construction, the Feynman/DeWitt–Morette representation, and its connection to a possible new class of stochastic processes. Finally, application to seismic imaging/inversion will be briefly addressed.

IC/MP160/010: Path integrals: classical waves, quantum waves, and modern mathematical asymptotics, I: phase-space constructions, convergence issues, and seismic and electromagnetic applications. #2

Organiser: Bair Budaev (University of California, Berkeley, USA)
Co-organiser: Louis Fishman (MDF International, USA)

(For abstract, see session #1 above.)

FIO-product representation of solutions to symmetrizable hyperbolic systems. **Jérôme Le Rousseau** (Université de Provence Aix-Marseille I, France) IC/MT2653/010

Let $n, k \in \mathbb{N}^*$. We consider a first-order Cauchy problem:

$$\partial_z u + a(z,x,D_x)u = 0\,, \tag{1}$$

$$0 < z \le Z \;u\,|_{z=0} = u_0\,, \tag{2}$$

with $Z > 0$ and $a(z,x,\xi)$ a $k \times k$ matrix with entries continuous with respect to z with values in $S^1(\mathbb{R}^n \times \mathbb{R}^n)$ and $u = (u_1, \ldots, u_k)^t$, with the usual notation $D_x = \frac{1}{i}\partial_x$.

The matrix symbol $a(z,x,\xi)$ is assumed symmetrizable, in the sense that

$$a_1(z,x,\xi) = L(z,x,\xi)\alpha_1(z,x,\xi)(L(z,x,\xi))^{-1},$$

where $L(z,x,\xi)$ is a $k \times k$ invertible matrix with Lipschitz regularity with respect to z with values in $S^0(\mathbb{R}^n \times \mathbb{R}^n)$, and $\alpha_1(z,x,\xi)$ decomposes into $\alpha_1(z,x,\xi) = -i\beta_1(z,x,\xi) +$

$y_1(z,x,\xi)$ where both β_1 and y_1 are $k\times k$ Hermitian matrices that commute and can be smoothly diagonalized (e.g. in the case of constant multiplicities). We require $y_1(z,x,\xi)\geq 0$. The Cauchy problem is then hyperbolic and well-posed, with the initial data u_0 in any Sobolev space.

We define the *thin-slab* propagator, $\mathcal{G}_{(z',z)}$, $0\leq z\leq z'\leq Z$, to be the operator with kernel

$$G_{(z',z)}(x',x) := \frac{1}{(2\pi)^n}\int e^{i\langle x'-x|\xi\rangle}e^{-\Delta a_0(z,x,\xi)}e^{-\Delta a_1(z,x',\xi)}\mathrm{d}\xi,$$

with $\Delta = z'-z$, and prove it is a Fourier integral operator (FIO) with matrix phase of order 0.

We introduce the following Ansatz to approximate the solution operator: for $\mathfrak{P}=\{z^{(0)},z^{(1)},\dots,z^{(N)}\}$ a subdivision of $[0,Z]$ with $0=z^{(0)}<z^{(1)}<\cdots<z^{(N)}=Z$ such that $z^{(i+1)}-z^{(i)}=\Delta_{\mathfrak{P}}$, the operator $\mathcal{W}_{\mathfrak{P},z}$ is

$$\mathcal{W}_{\mathfrak{P},z} := \begin{cases} \mathcal{G}_{(z,0)} & \text{if } 0\leq z\leq z^{(1)},\\ \mathcal{G}_{(z,z^{(k)})}\prod_{i=k}^{1}\mathcal{G}_{(z^{(i)},z^{(i-1)})} & \text{if } z^{(k)}\leq z\leq z^{(k+1)}. \end{cases}$$

Let $s\in\mathbb{R}$ and assume $u_0\in(H^{(s+1)}(\mathbb{R}^n))^k$. We prove that, if the matrix symbol $a(z,.)$ is of Hölder regularity with respect to z, the Ansatz $\mathcal{W}_{\mathfrak{P},z}$ converges to the solution operator, $U(z,0)$, of the Cauchy problem (1)-(2) in operator norm in $L((H^{(s+1)}(\mathbb{R}^n))^k,(H^{(s+r)}(\mathbb{R}^n))^k)$ as $\Delta_{\mathfrak{P}}$ goes to 0 with a convergence rate of order $\alpha(1-r)$, $0\leq r<1$,

$$\|\mathcal{W}_{\mathfrak{P},z}-U(z,0)\|_{((H^{(s+1)})^k,(H^{(s+r)})^k)}\leq C\Delta_{\mathfrak{P}}^{\alpha(1-r)},\quad z\in[0,Z].$$

In the case $r=1$ we have strong convergence. The solution to (1)-(2) can thus be written as the result of the action of an infinite product of FIOs on u_0.

We shall connect this result with path integration and will provide applications and numerical examples in seismology.

Feynman operator calculus on Banach spaces I: basic theory. **Tepper Gill** (Howard University, USA) IC/MT3385/010

In order to extend our constructive representation theory of Feynman's operator calculus to Banach spaces, we use a result of Gross and Kuelbs, which shows that all separable Banach spaces may be rigged between two Hilbert spaces as dense continuous embeddings. We then construct continuous tensor product Banach spaces along the lines used by von Neumann to construct continuous tensor product Hilbert spaces. We then present a number of new results on operator extensions, which allow us to lift our representation theory from the Hilbert space to the Banach space setting. We then construct time-ordered integrals for general contraction semigroups.

Feynman operator calculus on Banach spaces II: generation theory. **Woodford Zachary** (Howard University, USA) IC/MT3380/010

We provide a general theory of time-ordered evolution operators on Banach spaces. First, we extend the general theory of operator semigroups to the time-ordered setting and prove a few of the generation theorems, including the famous Hille-Yosida Theorem. We then unify the theory of time-dependent hyperbolic and parabolic evolution equations. We extend the Dyson expansion to the Banach space setting and provide a general theory for the interaction representation of relativistic quantum theory. In addition, we provide a strong generalization of the Feynman-Kac formula for path integrals on Banach spaces.

IC/MP320/015: Non-local electrostatic effects in liquid crystals: fibers and elastomers.

Organiser: Carme Calderer (University of Minnesota, USA)
Co-organiser: Patricia Bauman (Purdue University, USA)
Co-organiser: Daniel Phillips (Purdue University, USA)

In the last decades, optic applications of nematic liquid crystals have met an enormous success in display manufacturing, including large video devices. This motivated a lot of activity in the mathematics community, especially in studies of calculus of variations, defects and flow problems.

The discovery and synthesis of new types of liquid crystals has also brought up new questions in modeling and analysis. New materials include the molecular *banana-shape* liquid crystals and the elastomers. The former are characterized by the ferroelectric behavior and belong to the class of smectic phases, with higher ordering than nematic. This combined with their liquid nature results in their manifestation as filaments of complicated shapes and respond to electric fields in a nonlocal fashion.

Liquid crystal elastomers are solids that combine mathematical features of nonlinear elasticity and those of standard liquid crystals. In particular, their gel states are of interest in application to soft tissue. Some of such materials are also biaxial in the bulk. The presentations will deal with models and analysis of ferroelectricity, biaxiality, filament stability, elastomers and gel states. One of the lecutures will address the optic properties of negative index materials found in chiral liquid crystals.

Stable bent-core liquid fibers. **Daniel Phillips** (Purdue University, USA) IC/MT3336/0

We consider a model for drawn fibers formed from cylindrical, smectic layers of banana-shaped liquid-crystal molecules. The molecules' shape induces both a spontaneous polarization and a distinctive effect on layer density. These features lead to a model that predicts stable fiber formation. We analyze solutions from this model and their electro-magnetic properties. This is joint work with C. Bailey, P. Bauman, and C.Calderer.

Adaptive-grid methods for Q-tensor theory of liquid crystals. **Alison Ramage** (University of Strathclyde, UK) IC/MT3681/015

In addition to the defect core structure, the dynamics of defect movement is also a crucial issue for liquid crystal cells. Previous numerical simulations of such effects have mostly involved using standard finite difference or finite element techniques on uniform grids, and have often been based on using director theory rather than the $\mathbf{Q}$-tensor approach proposed here. However, the presence in the physical problem of characteristic lengths with large scale differences (the size of the defect is very small compared to that of the cell) suggests that more sophisticated numerical modelling techniques could be used to great effect. One obvious approach is to use an adaptive grid technique, ensuring that there is no waste of computational effort in areas where there is no need for a fine grid. Adaptive grid methods have been successfully used to solve PDEs in many branches of computational mathematics such as computational fluid dynamics, mathematical biology, semiconductor modelling and aerospace engineering. In this talk we will present an introductory study of the use of adaptive grid methods for solving PDE problems in $\mathbf{Q}$-tensor theory of liquid crystals. This work is in collaboration with Dr Christopher J. Newton of Hewlett-Packard Laboratories in Bristol, UK.

Landau–de Gennes theory of isotropic–nematic–smectic liquid crystal transitions. **Paolo Biscari** (Politecnico di Milano, Italy) IC/MT3744/0

We propose a new version of Landau-de Gennes variational theory fit to simultaneously describe isotropic, nematic, smectic-A, and smectic-C phases of a liquid crystal. The unified description allows us to deal with systems in which one, or all, of the order parameters develop because of the influence of defects, external fields and/or boundary conditions. We derive the complete phase diagram of the system, that is, we characterize how the homogenous minimizers depend on the value of the constitutive parameters. The coupling between the nematic order tensor and the complex smectic-A order parameter generates an elastic potential which is a non-convex function of the gradient of the smectic order parameter. This lack of convexity yields in turn a loss of regularity of the free-energy minimizers. We then consider the effect on an infinitesimal second-order regularization term in the free-energy functional, which fixes the optimal number of defects in the singular configurations.

IC/MP320/015: Non-local electrostatic effects in liquid crystals: fibers and elastomers. #2

Organiser: Carme Calderer (University of Minnesota, USA)
Co-organiser: Patricia Bauman (Purdue University, USA)
Co-organiser: Daniel Phillips (Purdue University, USA)

(For abstract, see session #1 above.)

Swelling dynamics of nematic elastomers. **Peter Palffy-Muhoray** (Kent State University, USA) IC/MT4190/0

Liquid crystal elastomers (LCEs) are exceptionally responsive materials due to the coupling of orientational order and mechanical strain. Changes in orientational order due to thermal, electric, magnetic or chemical excitations can give rise to mechanical deformations. Swelling LCEs with solvents differs from that of isotropic rubbers in that changes in orientational order due to the presence of the solvent contribute significantly to changes in sample shape, giving rise to unusual behavior. We present some results of experiments on swelling monodomain nematic LCE samples with liquid solvents, solvent mixtures and solvent vapors, and discuss the observed excitation and relaxation dynamics. We briefly describe a continuum model, combining features of liquid crystallinity, binary mixtures and elasticity, proposed to describe this behavior. We conclude by considering the potential of the chemical response of LCEs for applications in devices such as chemical sensors, switches and motors. This work was done in collaboration with A. Golemme, T. Toth-Katona, M. Shelley and M Warner.

Effective models for nematic liquid crystals with ferromagnetic inclusions. **Dmitry Golovaty** (The University of Akron, USA), Carme Calderer (University of Minnesota, USA), Antonio DeSimone (SISSA, Trieste, Italy), Alexander Panchenko (Washington State University, USA) IC/MT4193/0

We use the methods of the theory of homogenization to establish the effective models for ferronematics - magnetic suspensions of needle-like particles in a nematic liquid-crystalline matrix. When the volume fraction of slightly prolate spheroidal particles is small, we show that the effective energy functional is essentially the same as the standard Oseen-Frank energy, however the coefficient in front of the term coupling the nematic director to the applied field is much larger than that for the pure nematic. Further, we discuss the influence of the interplay between the elastic/anchoring properties of the nematic, aspect ratio of the particles, and the volume fraction of the particles on characteristics of the effective medium.

Energy minimization and orientability for planar nematic liquid crystals. **Arghir Zarnescu** (University of Oxford, UK), John Ball (University of Oxford, UK) IC/MT5061/015

The Oseen–Frank theory is the model which has been most studied mathematically among those attempting to describe uniaxial nematic liquid crystals. It represents the liquid crystals by means of unit length vector fields describing the local mean orientation of molecules. An apparent deficiency of the Oseen-Frank theory is that is does not recognize the "head-to-tail" symmetry of the physical system. This symmetry is respected by the (constant order parameter) Landau-de Gennes Q-tensor theory, which uses line fields instead of vector fields. A vector field can be reduced to a line field but not necessarily the other way around. There exist line fields that cannot be "oriented" into vector fields, without creating discontinuities. We call such line fields non-orientable. We analyze, in a 2D geometry, the circumstances in which the non-orientable line fields are energetically favoured over the orientable ones. Thus we identify the instances in which the Oseen-Frank theory fails to recognize the correct, physical, energy minimizers.

IC/MP622/131: Inverse problems in electromagnetic scattering.

Organiser: Dietmar Hömberg (Weierstraß-Institut Berlin, Germany)
Co-organiser: Markus Bär (PTB-Berlin, Germany)

Electromagnetic scattering and diffraction in complex geometries are of great relevance to many application in material science and precision measurement. Examples include metamaterials, photonic crystals as well as methods to determine structural properties from indirect measurement e. g. in scatterometry where UV light is scattered at nanostructured functional elements commonly used in microelectronics. In the latter case, the scattering signature is used to reconstruct the geometrical profile of periodic gratings. This process requires the solution of a difficult and computationally intensive inverse problem that involves detailed mathematical analysis as well as efficient numerical procedures. This minisymposium gives an overview of modern application of inverse problems in electromagnetic scattering and addresses issues such as sensitivity analysis, state-of-the art treatment of boundary conditions as well as fast solvers for Maxwellt's equations.

On the direct and inverse problems in fluid–structure interaction. **George Hsiao** (University of Delaware, USA) IC/MT2598/131

This lecture is based on joint work with J. Elschner and A. Rathsfeld of WIAS in Berlin, and it is concerned with the direct and inverse scattering problems in fluid–structure interaction. The scattering problem in the fluid–structure interaction can be simply described as follows: an acoustic wave propagates in the fluid domain of infinite extent where a bounded elastic body is immersed. The direct problem is to determine the scattered pressure and velocity fields in the fluid domain as well as the displacement fields in the elastic body, while the inverse problem is to reconstruct the shape of the elastic scatterer from a knowledge of the far field pattern of the fluid pressure or from the measured scattered fluid pressure field. As is well known, the inverse problems are generally nonlinear and highly ill-posed. For treating inverse problem of this kind, we reformulate the problem as a nonlinear optimization problem including special regularization terms. The precise formulation of the nonlinear objective functional will depend on the approaches of the direct problem. In this lecture we will present various approaches for the direct problem based on the formulations with or without introducing artificial boundaries and their corresponding formulations of the inverse problem. Emphasis will be placed upon the mathematical foundations of the variational formulations of the corresponding problems.

Sensitivity analysis for indirect measurement in scatterometry and the reconstruction of periodic-grating structures. **Andreas Rathsfeld** (Weierstraß-Institut Berlin, Germany), Hermann Gross (PTB-Berlin, Germany) IC/MT1243/131

We discuss numerical algorithms for the determination of periodic surface structures from light diffraction patterns. With decreasing details of lithography masks, increasing demands on metrology techniques arise. Scatterometry as a non-imaging indirect optical method is applied to simple periodic line structures in order to determine parameters like side-wall angles, heights, top and bottom widths and to evaluate the quality of the manufacturing process. The numerical simulation of diffraction is based on the finite element solution of the Helmholtz equation. The inverse problem seeks to reconstruct the grating geometry from measured diffraction patterns. Restricting the class of gratings and the set of measurements, this inverse problem can be reformulated as a non-linear operator equation in Euclidean spaces. The operator maps the grating parameters to special efficiencies of diffracted plane wave modes. We employ a Gauß-Newton type iterative method to solve this operator equation. The reconstruction properties and the convergence of the algorithm, however, is controlled by the local conditioning of the non-linear mapping. To improve reconstruction and convergence, we determine optimal sets of efficiencies optimizing the condition numbers of the corresponding Jacobians. Numerical examples for chrome-glass masks and for inspecting light of wavelength 632.8 nm are presented.

Lithography mask characterization from measured scatterometry data. **Frank Schmidt** (Zuse-Institut Berlin, Germany), Burger Sven (Zuse-Institut Berlin, Germany), Jan Pomplun (Zuse-Institut Berlin, Germany), Lin Zschiedrich (Zuse-Institut Berlin, Germany) IC/MT2682/131

Progress in development of smaller and faster computers is connected to decreasing size of geometrical structures of microchips. Extreme ultraviolet (EUV) lithography is seen as the main candidate for further miniaturization of computer technology. Due to the short wavelength of EUV light (≈ 13 nm) novel reflective EUV masks have to be used in the production process.

EUV masks have geometrical feature sizes of the order of the wavelength of EUV light and are illuminated at oblique incidence. Therefore the quality of pattern profiles of EUV masks becomes very important and has to be controlled.

To simulate light propagation in EUV masks we have to solve Maxwell's equations. For this purpose we have developed an adaptive finite element (FEM) approach on irregular meshes [1]. The usage of irregular triangulations allows us to accurately model the geometry of EUV masks. Special domain decomposition techniques [2] significantly decrease computational time and increase accuracy. These are crucial points for reconstruction of mask parameters from experimental data.

Here we present rigorous simulations of EUV masks with different geometrical mask parameters like side-wall angles, corner roundings, layer heights and widths. We optimize the geometry of simulated EUV masks to fit numerical results to data obtained from experimental scatterometry [3]. The obtained geometrical parameters from this indirect metrology technique are compared to direct quantitative microscopy of EUV mask patterns and show good agreement.

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Stochastic characterization of non-stationary over-moded fields. **Luk Arnaut** (National Physical Laboratory, UK) IC/MT2205/131

We investigate the effect of rapid variations of cavity boundaries on the dynamic and stochastic properties of a nonstationary electromagnetic field inside a reverberant enclosure. This case constitutes a generalization of an idealized statistically incoherent, homogeneous, isotropic, quasi-static, random vector field, which is retrieved as a special case. A theoretical model is constructed to show how the field can be characterized as a generalized wave diffusion process. The Langevin–Ito and Fokker–Planck equations, distributions and statistics for the instantaneous field, its magnitude and energy density are derived and solved analytically. The results have applications, in particular, for the characterization of multipath propagation of electromagnetic waves in complex and dynamic environments exhibiting time-varying multiple scattering.

IC/MP250/131: Nonlinear dynamics in lasers.

Organiser: Nathan Kutz (University of Washington, USA)

Mode-locked lasers are one of the most successful commercial devices which are based fundamentally on nonlinear optics. Commercially available pulsed mode-locked lasers are compact, cheap, reliable and robust and have a wide range of applications from optical communications to medical devices. Thus considerable interest and research in the past decade has focused on the use of Erbium-doped fibers in actively and passively mode-locked fiber lasers operating in both the normal and anomalous dispersion regimes. Many mode-locking schemes have been successfully demonstrated. These include active mode-locking with an acousto-optic modulator, passive mode-locking via nonlinear interferometry in the figure eight laser, polarization rotation in the ring laser, and a linear cavity configuration which employs a semiconductor structure for fast saturable absorption. A generic feature of each mode-locked laser is the intensity-dependent loss which is achieved by the mode-locking mechanism. The additional loss imparted upon low-intensity parts of the pulse, whether it

be dispersive radiation or the wings of a pulse, gives the necessary pulse shaping required to achieve stable mode-locking operation. These compact sources of optical pulses near wavelengths of 1.55 microns are key enabling technologies for high speed fiber optic communication systems and interconnection networks.

Accurate modeling of these technologically promising mode-locked fiber lasers is essential to their utilization in practical systems. Many models have been developed which attempt to address various aspects of the mode-locking dynamics ranging from the energy equilibration in the cavity to the polarization dynamics of the pulse and the pulse-to-pulse interactions in a harmonic mode-locking configuration. Each model has merit in describing a certain aspect of the laser dynamics, and it is difficult to develop a single model which encompasses all aspects of the mode-locking dynamics. In this mini-symposia, a variety of mathematical models are presented which address the variety of phenomena observed in laser systems. Special attention is given to the role of nonlinearity in determining the fundamental dynamical behavior in the laser cavity which includes its stability, bifurcation structure, and onset of chaos.

Delay-coupled laser systems: scaling laws and resonances. **Thomas Carr** (Southern Methodist University, USA) IC/MT3562/131

We consider a model for two lasers that are mutually coupled optoelectronically by modulating the pump of one laser with the intensity deviations of the other. Signal propagation time in the optoelectronic loop causes a significant delay leading to the onset of oscillatory output. Multiscale perturbation methods are used to describe the amplitude and period of oscillations as a function of the coupling strength and delay time. Because we allow for independent control of the individual coupling constants, for certain parameter values there is an atypical amplitude-resonance phenomena. Our theoretical results are consistent with recent experimental observations when the inclusion of a low-pass filter in the coupling loop is taken into account.

Mode-locking via nonlinear mode-coupling: global attractors. **Joshua Proctor** (Princeton University, USA) IC/MT4712/131

A detailed analysis of mode-locking is presented in which the nonlinear mode-coupling behavior in a waveguide array, dual-core fiber, and/or fiber array is used to achieve stable and robust passive mode-locking. By using the discrete, nearest-neighbor spatial coupling of these nonlinear mode-coupling devices, low-intensity light can be transferred to the neighboring waveguides and ejected (attenuated) from the laser cavity. In contrast, higher intensity light is self-focused in the launch waveguide and remains largely unaffected. This nonlinear effect, which is a discrete Kerr lens effect, leads to the temporal intensity discrimination required in the laser cavity for mode-locking. Numerical studies of this pulse shaping mechanism show that using current waveguide arrays, fiber-arrays, or dual-core fibers in conjunction with standard optical fiber technology, stable and robust mode-locked soliton-like pulses which act as global attractors are produced.

Multi-frequecy mode-locked lasers. **Edward Farnum** (Kean University, USA) IC/MT4707/131

A new theoretical model is constructed which describes the operation of multi-frequency, pulsed mode-locked laser cavities. The model, which is a combination of multi channel interactions in the canonical master mode-locking model subject to three different gain models which account for both self- and cross-saturation effects, results in mode-locking dynamics which qualitatively describe the observed experimental dual-frequency laser operation. Specifically, the combination of self- and cross-saturation in the gain allows for mode-locking at two frequencies simultaneously, which can be of significantly different energies and pulsewidths. The model gives a framework for understanding the operation and stability of the increasingly important and timely technology of dual- and multi-frequency mode-locked laser cavities.

Dissipative solitons and their interactions. **Nail Akhmediev** (Australian National University) IC/MT3859/131

Coupled soliton pairs in nonlinear dissipative systems can exist in various forms. They can be stationary, or they can pulsate periodically, quasi-periodically or chaotically, as is the case for single solitons. Each type is stable in the sense that a given bound state exists in the same form indefinitely. Single solitons can be perfectly stable for a given set of parameters. However, this does not mean that a bound state formed from them is either stationary or stable. Moreover, their relations can be highly complicated. Such is the life of dissipative solitons.

IC/MP293/132: Mathematical and numerical modeling of quantum transport in nano-structures.

Organiser: Florian Méhats (Université de Rennes 1, France)
Co-organiser: Pierre Degond (Université Paul Sabatier Toulouse III, France)

Improving information and communication technologies relies among others on the design of ultra high-speed and low-consumption electronic devices. This goal requires the reduction of device sizes up to the nanometer scale or even the atomic one. At such scales, quantum interference, tunneling and confinement play an important role and have an extremely high impact on device operation. They can even represent, like in resonant tunneling diodes, the major effects governing the electronic transport. The aim of the minisymposium is to provide an overview of recent developments concerning the mathematical and numerical modeling of quantum transport in nanostructures. The topics will emphasize industrial challenges in the area, the physical important effects and the mathematical modeling and simulation issues related to them, and we will focus on the interplay between physical, engineering and mathematical aspects. Quantum transport in nanostructures can be modeled through a variety of models adapted to different physical situations. At the microscopic level, the Schrödinger equation (or its reformulation using the Green's functions method) can be employed in order to describe ballistic regimes. When the transport is more collisional, a solution consists in using the phase-space counterpart of the Schrödinger equation, the Wigner equation, and taking into account collision effects through Boltzmann type kernels. Such systems are often treated with Monte-Carlo methods. However, these models may be computationnally expensive and a recent area of research consists in the derivation of quantum hydrodynamical systems, in order to describe the system at a macroscopic scale. This minisymposium will propose four talks covering several levels of modeling, from the microscopic to the macroscopic level of description.

Quantum corrected drift-diffusion models: solution fixed-point map and finite-element approximation. **Riccardo Sacco** (Politecnico di Milano, Italy), Joseph Jerome (Northwestern University, USA), Carlo de Falco (Bergische Universitaet Wuppertal, Fachbereich C -, Germany) IC/MT1084/132

In this lecture, we deal with the analysis of the functional iteration proposed in[2] for the decoupled solution of the Quantum Drift-Diffusion (QDD) model. The functional iteration is denoted Generalized Gummel Map, because it is a consistent generalization to the quantum-corrected setting of Gummel's iterative procedure, widely used in contemporary semiconductor simulation based on the DD transport model. The ideas developed in this lecture try to combine the main results of the existence analysis carried out in[1] for the QDD model, with the corresponding analysis of the solution map carried out in[3] in the case of the DD model. It is expected that, with some modifications, the proposed theoretical framework can be extended to deal with other quantum-corrected models, as considered in[2].

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Quantum dynamics of ultrafast photoinduced processes in organic semiconductor systems. **Irene Burghardt** (École Normale Supérieure de Paris, France) IC/MT3147/132

The photophysics of π-conjugated organic semiconductor systems is a key ingredient in the technological development of optoelectronic devices. Due to their spatially extended structure, these systems exhibit both the molecular characteristics of their components and the collective electronic excitations (exciton states) characteristic of lattice structures. The coupling between electronic and nuclear motions results in the localization ("self-trapping") of exciton states, along with the coherent nuclear dynamics and vibronic coupling phenomena known from molecular systems. Of particular interest are ultrafast exciton dissociation processes at polymer heterojunctions, comprising two materials with an offset between the constituent valence and conduction bands [1]. For these systems, the non-adiabatic coupling between the initially excited exciton state and a localized charge transfer state plays a key role. As we have recently shown, the subpicosecond scale dynamics of exciton dissociation is indeed essentially of non-adiabatic nature [2,3]. In this presentation, we report on quantum-dynamical simulations of this process using efficient multiconfigurational techniques [2]. We further provide a perspective on the combined description of exciton creation, migration, and localization phenomena in conjunction with quantum non-adiabatic transitions.

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Towards high-fidelity large-scale atomistic simulations of emerging materials and electronic devices. **Eric Polizzi** (University of Massachusetts, USA) IC/MT3225/132

In nanoscience research, numerical simulations are vital in focusing experimental investigation for the exploration of new classes of high speed, and high functionality devices. Characterization of nanoscale emerging devices needs to be addressed via reliable, robust and accurate quantum simulations. As a result, comprehensive and realistic electronic structure and electron transport simulations need to account for: (i) information of the material at the atomistic level, (ii) multiscale aspects of electron transport modeling and electrostatics effects, (iii) high-fidelity treatment of the contact regions, and (iv) efficient methodology for dissipative scattering. The quest for ever higher levels of detail and realism in these simulations presents formidable modeling and computational challenges. These nanoelectronics simulations are expected, however, to benefit from the development of specific advanced mathematical techniques and high-performance parallel algorithms to enhance our ability to achieve high-fidelity simulations of materials and transport problems. Here, we propose to investigate novel simulation strategies which aim to go beyond qualitative predictions by proposing quantitative simulations from the atomistic scale to the transistor macroscale.

Quantum Monte-Carlo methods based on a multi-scale approach. **Christian Ringhofer** (Arizona State University, USA) IC/MT3027/132

Quantum mechanical transport phenomena are included into semi-classical Monte Carlo methods for electron gases in a multi - scale framework. The small scale transport picture is based on a general framework to derive macroscopic transport equations for a small set of observables based on maximum entropy closures.

13: Physics and Electrical Engineering, Contributed Talks

IC/CTS4902/13: **Physics and electrical engineering.**

Organiser: Marissa Condon (Dublin City University, Ireland)
Co-organiser: James Gleeson (University College Cork, Ireland)

Numerical modelling of flow plasma interactions. **Guillaume Dufour** (ONERA, France), Francois Rogier (ONERA, France) IC/CT1116/013

This paper deals with the numerical modeling of plasma flow interactions at atmospheric pressure and their application to aeronautics. A two-dimensional air plasma modeling including complex air kinetic and flow motion, coupled with the evolution of the generated electrical field, is proposed to describe the plasma creation. The net force exerted by the plasma on the flow is then computed and introduced in a Navier-Stokes solver in order to evaluate its influence on the air flow. The presented model is able to compute pin plate coronas discharges as well as wire to wire ones so that a wide panel of experimental setups is covered. The cornerstone of plasma discharges simulation is the ability to deal with multiscale physical phenomena (the kinetic dynamic is much steeper than the transport of the ions, for example). The objective is then to avoid the limitation imposed by the steepest phenomenon and to reduce the computational time (and cost). In this paper, some numerical methods to overcome this kind of difficulties are presented and the opportunity to use surrogate models is discussed. Finally, numerical simulations are performed for a corona wire to wire discharge and the numerical results obtained are compared with LEA experimental ones, thus emphasizing the ability of the model to predict the correct behaviour of the discharge.

Model reduction of nonlinear systems. **Marissa Condon** (Dublin City University, Ireland) IC/CT399/133

As the accuracy and complexity of the mathematical models that describe dynamical systems grows, the consequence unfortunately is a result in increased computation time and use of computer memory resources. However, in many engineering applications, for example, in controller design for aeronautics or for testing the functionality of an initial RF system design, only the essential behaviour of a system is required. Furthermore repeated iterations are required to identify and select a suitable design. Hence, there is a need to formalise techniques for the accurate formation of reduced-order models to enable rapid repetitive or iterative simulation. While numerous effective techniques exist for linear model reduction, the procedure for nonlinear model reduction is far more complex. With nonlinear predictive control methods or with nonlinear problems associated with analog circuitry or micromachined devices, however nonlinear model reduction has become of paramount importance. In this talk, we will give an overview of the significant procedures for nonlinear model reduction employed at present. In particular, we will look at the general merits and demerits of methods based on balanced truncation and methods based on Krylov approaches. Specifically, we will explore empirical balanced truncation and the use of algebraic gramians for the former method. We will look at projection methods or Krylov approaches in relation to polynomial expansions and bilinear approximations. We will then focus on the perturbative representation of the nonlinear system. We will apply a novel model reduction technique to this representation and explore its use in conjunction with other methods. We will consider a standard test case for comparing the various methods. The efficacy of the novel method will be highlighted.

New finite elements for large-scale simulation of optical waves. **Britta Heubeck** (Universität Erlangen–Nürnberg, Germany), Christoph Pflaum (Universität Erlangen–Nürnberg, Germany), Gunther Steinle (Infineon Technologies AG, Germany) IC/CT4334/131

We present a new technique for the time-dependent simulation of the optical wave and the carrier density in Distributed Feedback (DFB) lasers. The time-dynamic behaviour is simulated by rate equations. These rate equations consist of three coupled partial differential equations: While the optical wave is described by the time-dependent Helmholtz equation, the carrier density is specified by the drift-diffusion equation. This is a pair of coupled partial differential equations characterizing the carrier density in the active zone and within the barriers. Our goal is to solve these rate equations for DFB lasers. As such lasers consist of a long resonator compared to the wavelength of laser light, problems arise when solving this system numerically. Standard finite element methods cannot be applied, as for resolving the wave appropriately, a huge amount of grid points is needed. Furthermore, the Beam Propagation Method is not suitable, as by this method it is difficult to simulate internal reflections.

We propose a new finite element method for solving the two-dimensional Helmholtz resonator equation on long geometries. This method is based on newly developed Trigonometric Finite Wave Elements (TFWE) constructed by linear elements and trigonometric functions. We compare this so-called TFWE Method to common techniques like the Transfer Matrix Method and present numerical results that demonstrate the superiority of our method. Furthermore, our approach requires less grid points compared to standard finite elements since the TFWE lead to a more accurate approximation of the optical wave. Thus, we get a smaller linear system of equations which eases the solving process. Another advantage is that the TFWE simplify the modelling of boundary conditions (bc), in particular of the absorbing bc. The TFWE Method can also be applied to two-dimensional configurations when other methods fail. Finally, typical experimental lasing effects, e.g. spatial hole burning, can be simulated.

Performance of various block preconditioners for FEM modeling of semiconductor devices. **Paul Lin** (Sandia National Laboratories, USA), John Shadid (Sandia National Laboratories, USA), Robert Hoekstra (Sandia National Laboratories, USA), Gary Hennigan (Sandia National Laboratories, USA) IC/CT2522/132

Approximate block factorization preconditioners are applied to the drift-diffusion equations for modeling semiconductor devices. The block factorization essentially produces a "physics-based" preconditioner for the drift-diffusion system. The system is comprised of a nearly singularly perturbed elliptic constraint for the electric potential, and two parabolic convection-diffusion-reaction equations for the electron and hole concentrations. The resulting scalar subsystems are solved by various iterative methods including AMG-type techniques. We demonstrate these techniques by employing a stabilized finite element discretization of the drift-diffusion equations on structured and unstructured meshes. The nonlinear coupled system is solved with a parallel preconditioned Newton-Krylov method. Preliminary results will be presented demonstrating the performance of the approximate block factorization preconditioners compared with one-level and multilevel domain decomposition preconditioners. This work was partially funded by the DOE NNSA's ASC Program and the DOE Office of Science AMR Program, and was carried out at Sandia National Laboratories operated for the U.S. Department of Energy under contract no. DE-ACO4-94AL85000

Sorting of microparticles in periodic and random potentials. **James Gleeson** (University College Cork, Ireland) IC/CT1938/010

There has been a recent revolution in the ability to manipulate micrometer-sized objects on surfaces patterned by traps or obstacles of controllable configurations and shapes. One application of this technology is to separate particles driven across such a surface by an external force according to some particle characteristic such as size or index of refraction. The surface features cause the trajectories of particles driven across the surface to deviate from the direction of the force by an amount that depends on the particular characteristic, thus leading to sorting. While models of this behavior have provided a good understanding of these observations, the solutions have so far been primarily numerical. In this work we provide analytic predictions for the dependence of the angle between the direction of motion and the external force on a number of model parameters for periodic as well as random surfaces. We test these predictions against exact numerical simulations.

Work done in collaboration with: J. M. Sancho (Universitat de Barcelona), A. M. Lacasta (Universitat Politecnica de Catalunya, Barcelona), and Katja Lindenberg (University of California, San Diego).

IC/CTS4901/13: Electromagnetics and photonics.

Organiser: Ya Yan Lu (City University of Hong Kong)
Co-organiser: Vincent Mazauric (Schneider Electric, France)

A global approach of electromagnetism dedicated to further long-term planning. **Vincent Mazauric** (Schneider Electric, France), Nadia Maïzi (Ecole des Mines de Paris, France) IC/CT3347/131

In order to provide a vision of power electrical engineering for future energy-supply crossroads and sustainable challenges, quasi-static laws of electromagnetism are deduced from experimental evidences, the electric charge conservation and variational principles derived from thermostatistics. While flux-density divergence free is obtained everywhere from the stationary condition on the Gibbs' free energy, the Maxwell-Faraday equation and the Ohm's law with motion are obtained in conductors by assuming a trend for a reversible evolution of the electromagnetic field. In other words, the local laws of electromagnetism may be obtained from an optimization of the global mechanical power exchanged throughout the electrical network. The approach is shown to be: (i) consistent with Finite Element Method ; (ii) coherent with a coarse graining optimization, from scratch to the design scale ; (iii) suitable to consolidate energy processes involved in electromagnetic and electromechanical conversion. Hence, two kinds of devices are identified: (i) those dedicated to power conversion where the highest efficiency should be achieved; and their (ii) couplings involved in transmission lines, distribution busways, cablings and PCBs where the voltage does not drop. In spite of this ideal trend, an actual network undergoes irreversible processes for the length- and time-scales on which it is monitored. Usually, this lack of information is counteracted by the reactive energy for admissible load fluctuations. Hence, for a given level of reliability, the network management results from a compromise between: stock of reactive energy and investment for the monitoring and rush production capabilities. Such an approach should allow to improve the Life Cycle Assessment of the electrical supply-chain and consequently provide a description of power electrical engineering suitable for long-term planning.

A Dirichlet-to-Neumann map approach to photonic-crystal modeling. **Ya Yan Lu** (City University of Hong Kong) IC/CT1022/131

Photonic crystals are engineered material with periodic structures on the scale of a wavelength of the light. Due to the existence of photonic bandgaps (these are intervals of the frequency, such that light corresponding to a frequency in a bandgap cannot penetrate the photonic crystal), they could play a very important role in future integrated optical circuits, a role as semi-conductors in current electric integrated circuits. Mathematical modeling and numerical simulations of photonic crystals are challenging. Existing numerical methods that discretize the whole structure are not very efficient. We develop a special class of methods based on the Dirichlet-to-Neumann maps. The efficiency and accuracy of our methods are illustrated in numerical examples for computing the bandgaps, transmission spectra and waveguide modes of photonic crystals.

Optical solitons with dual power-law nonlinearity. **Anjan Biswas** (Delaware State University, USA) IC/CT1121/131

The multiple scale perturbation analysis is used to study perturbed optical solitons that are governed by nonlinear Schrödinger's equation with dual-power law nonlinearity. The perturbations due to nonlinear damping and saturable amplifiers are considered. This method obtains new results that are not recoverable by the traditional soliton perturbation theory.

Comparison of solution techniques for the linear system arising from the discretisation of time-harmonic scattering problems with $H(\mathrm{curl})$ elements. **Paul Ledger** (Swansea University, UK) IC/CT3737/131

This talk is concerned with approaches for the solution of the linear system of equation which arises when the vector wave equation for time harmonic scattering problems is discretised by $\vec{H}(\mathrm{curl})$ conforming finite elements on three–dimensional unstructured grids. The hp version of the finite element method is employed as it enables singularities to be captured without effecting smooth parts of the solution. In addition, a perfectly matched layer (PML) technique is used to truncate an otherwise infinite domain close to the scatterer.

The coefficient matrix which arises in this case is complex symmetric and indefinite. These properties are less than desirable and make this type of linear equation system notoriously difficult to solve. However, the structure of the coefficient matrix is sparse and contains many non zero entries and so may be stored efficiently. The actual dimension of the matrix depends on the level of refinement required for the problem being solved. One new emerging application is in the use of computational electromagnetics for cancer detection and for these problems the frequencies of interest are measured in microwaves. Using hp finite elements to solve time harmonic scattering problems at these frequencies translate to matrices which can readily be stored on a personal computer.

The computational performance of current direct and iterative solution strategies will be compared for a range of linear systems arising from the discrtisation of different problems. In particular, we shall investigate how well different preconditioners perform when applied to iterative solution algorithms. Possible modifications to the hp discretisation to facilitate easier linear equation solution will also be discussed.

Spectral filtering for ultra-short pulse generation in the normal (defocusing) dispersion regime . **Brandon Bale** (University of Washington, USA) IC/CT4733/010

Recent experiments show that ultra-short pulse generation can be obtained using a spectral filter in the normal dispersion regime of a laser cavity. The ratio of the width of the gain bandwidth to the width of the spectral filter is critical in determining the stability of the generated sinc-like mode-locked pulses. The spectral filtering allows one to obtain peak powers and pulse widths on the order of those achieved in the anomalous regime. We perform an extensive study of numerical and reduced models which characterize the stability and dynamics of the spectral filtering mode-locking process.

13: Physics and Electrical Engineering, Posters

IC/PP1100/010: Effect of dynamical cosmological constant in presence of modified Chaplygin gas for accelerating universe.

Presenter: Ujjal Debnath (Bengal Engineering and Science University, India)
Co-author: Writambhara Chakraborty (Kolkata, India)

In this paper we have considered the Universe to be filled with modified gas and the cosmological constant Λ to be time-dependent, with or without the gravitational constant G being time-dependent. We have considered various phenomenological models for Λ; viz., $\Lambda \propto \rho, \Lambda \propto \frac{\dot{a}^2}{a^2}$ and $\Lambda \propto \frac{\ddot{a}}{a}$. Using these models it is possible to show the accelerated expansion of the Universe at the present epoch. Also we have shown the natures of G and Λ over the total age of the Universe. Using the *statefinder* parameters we have shown the diagramamtical representation of the evolution of the Universe starting from radiation era to ΛCDM model.

IC/PP5056/131: Estimating the eddy-current modelling error.

Presenter: Kersten Schmidt (ETH Zürich, Switzerland)
Co-author: Oliver Sterz (Computer Simulation Technology, Germany)
Co-author: Ralf Hiptmair (ETH Zürich, Switzerland)

The eddy-current model is an approximation of the full Maxwell equations. We will give estimates for the modelling error and show how the constants in the estimates are influenced by the geometry of the problem. Additionally, we analyse the asymptotic behaviour of the modelling error when the angular frequency tends to zero. The theoretical results are complemented by numerical examples using high-order finite elements demonstrating that the estimates are sharp.

IC/PP4795/015: Computationally efficient simulation of polymer electrolyte fuel cells and stacks.

Presenter: Jens Eller (Zurich University of Applied Sciences Winterthur„ Switzerland)
Co-author: Markus Roos (Zurich University of Applied Sciences Winterthur„ Switzerland)
Co-author: Guido Sartoris (Zurich University of Applied Sciences Winterthur„ Switzerland)
Co-author: Jürgen Schumacher (Zurich University of Applied Sciences Winterthur„ Switzerland)

A computationally efficient model of a proton exchange membrane (PEM) fuel cell is presented. The approach is used for simulation of PEM single cells and stacks. In the framework of this "2+1D"-approach the anodic and cathodic fields are discretised in two dimensions with our finite element software SESES. The coupling between the anodic and cathodic side is established by a one-dimensional model representing the gas diffusion layer (GDL) and the membrane electrode assembly (MEA).

The nonlinear 1D model of the MEA and the GDLs is created by starting from the symbolic weak form expressions of the coupled transport phenomena. The tangential stiffness matrix of the coupled FEM problem is computed analytically by the computer algebra software Mathematica. As a next step a numerical FEM solution of the 1D model is calculated with Mathematica. Model validation is achieved by comparing the numerical 1D solution to spatially resolved current measurements with a fuel cell that is fed with pure oxygen. Finally, the validated 1D model of the MEA and the GDL is implemented with the programming language C and linked to SESES.

Coupling between the 1D model and the two 2D models in SESES is achieved by using the values of the degrees-of-freedom (DOF) variables of the 2D model as Dirichlet boundary conditions for the 1D model. The 1D model returns amendment for the right hand side of the solved governing equations in 2D computed as the non-zero residual at the 1D boundaries and their numerical derivatives with respect to the 1D Dirichlet boundary values.

This approach is suitable to take the high aspect ratio between the in-plane and the through-plane dimensions of fuel cells into account. The number of DOF variables is significantly reduced in comparison to a full 3D model approach. Further, this modelling approach can also be applied to other fields, e.g. for the description of coupled electro-chemical processes.

14: Computational Sciences, Minisymposia

IC/MP237/014: Problems involving interfaces: from models to computations.

Organiser: Georges-Henri Cottet (Université Grenoble I, France)
Co-organiser: John Strain (University of California, Berkeley, USA)

A number of computational problems in various applications critically involve interfaces. Whether they arise in e.g. mechanical engineering, physics or biomechanics, these problems share some common requirements:

- coupling between different types of physics and therefore different mathematical and numerical models, and
- capturing accurately a wide range of scales, in particular close to the interface.

Interfaces are often related to stability questions and numerical models must be able to distinguish between physical and numerical stability. Problems involving interfaces also require a choice between explicit interface tracking and implicit interface capturing.

This minisymposium will focus on several challenging applied problems where interfaces play a crucial role, in fluid dynamics, solid physics and fluid-structure interactions. The speakers will present state-of-the-art techniques, from model-oriented, mathematical and numerical points of view.

Pattern formation at the nano-scale in molecular beam epitaxy. **Olivier Pierre-Louis** (Université Joseph Fourier Grenoble, France) IC/MT2144/014

Molecular Beam Epitaxy is a major tool for the growth of atomically flat films. But a number of complex patterns are also observed during this type of growth. We here show how different techniques are used in order to determine the morphological evolution of the surface. We will analyze in more details the so-called phase field models. We will show how these models can either be (i) physical models, analogous to the phenomenological Ginzburg-Landau models; or (ii) tools for numerical simulations, which share similarities with level set models. Depending on the use which is made of the phase field, we will see how different constraints emerge on the formulation of the model.

Crystalline evolutions: a mathematical approach. **Matteo Novaga** (Università di Pisa, Italy) IC/MT768/014

I will discuss some aspects of motion by mean curvature of hypersurfaces in presence of nonsmooth anisotropies, including the so-called crystalline evolutions. I will give a survey of known results, and present some open problems.

Generalized Navier boundary condition for the numerical simulation of moving contact lines in two-fluid flows. **Jean-Frédéric Gerbeau** (INRIA Rocquencourt, France), Tony Lelièvre (École Nationale des Ponts et Chaussées, France) IC/MT810/014

We are interested in the numerical simulation of two incompressible viscous fluids separated by a free interface. We use an Arbitrary Lagrange Euler (ALE) formulation of the problem.

The purpose of the talk is to address various numerical issues, in particular some stability and conservation properties. The role of the Geometric Conservation Law (GCL) will be discussed. We will introduce a notion of *Surface Conservation Law* which may be helpful to analyse the numerical scheme when the surface tension is taken into account.

A difficult problem in the modelling of two-fluid flows in a bounded domain concerns the displacement of the contact line, namely the points which are at the intersection of the boundary of the domain and the interface separating the two fluids. We will show that variational formulations are well-suited to the *Generalized Navier Boundary Conditions* introduced by Qian, Wang and Sheng. Owing to these boundary conditions, it is possible to circumvent the incompatibility between the classical no-slip boundary condition and the fact that the contact line of the interface on the wall is actually moving. We will present numerical experiments on two-fluid flows in narrow channels and we will compare these results with molecular dynamics simulations from the literature.

Fast and accurate computation of layer heat potentials. **Jing Rebecca Li** (INRIA Rocquencourt, France), Leslie Greengard (Courant Institute, NYU, USA) IC/MT4982/014

We evaluate the single and double layer heat potentials in two dimensions on and off a moving boundary. The algorithm uses a high order quadrature in time which takes into account the integrable singularity at the endpoint as well as the smoothness of the integrand a short distance away. If a time quadrature point τ is close to the singularity, the spatial integral at τ is computed locally, using interpolated values. Otherwise it is computed using the Fast Gauss Transform. This algorithm can be used to compute the local part of layer potentials, in conjunction with the Fourier domain computation of the smooth part, while ensuring that the errors made in the local and the smooth parts are of a comparable magnitude. It can also be used adaptively to compute the full layer potential to a prescribed accuracy.

IC/MP237/014: Problems involving interfaces: from models to computations. #2

Organiser: Georges-Henri Cottet (Université Grenoble I, France)
Co-organiser: John Strain (University of California, Berkeley, USA)

(For abstract, see session #1 above.)

Bodies interacting with and through fluids. **Michael Shelley** (Courant Institute, NYU, USA) IC/MT2966/014

The interaction of flowing fluids with free bodies (sometimes compliant, sometimes active, sometimes multiple) constitutes a class of beautiful dynamic boundary problems that are central to biology and engineering. Examples range from how organisms locomote in fluids (which depends strongly on scale) to how non-Newtonian stresses develop in complex liquids (strongly dependent on the nature of fluidic microstructure). I will discuss several interesting examples, emphasizing how they are formulated mathematically so as to yield models tractable for analysis or simulation, and show how this work has interacted with experimental studies.

New methods in fluid-structure coupling with application to biomechanics. **Emmanuel Maitre** (Université Grenoble I, France), Georges-Henri Cottet (Université Grenoble I, France), Thomas Milcent (Université Grenoble I, France) IC/MT3499/014

An eulerian approach is presented for generic fluid-structure coupling of an elastic body with an incompressible fluid. We consider the coupling as a multiphysics problem where fluid-solid interfaces are captured by a level-set method. The main features of the method are its simplicity, and its natural control of mass and energy. We are indeed able to prove an energy equation which ensures in particular that the regularization of the force does not involve any energy dissipation. Applications to membranes oscillation and cardiomyocyte contraction are presented.

Locally-corrected semi-Lagrangian methods for Stokes flow with moving elastic interfaces. **J Thomas Beale** (Duke University, USA) IC/MT2542/014

We describe a numerical method developed in work with J. Strain for computing time-dependent viscous flow with a moving interface which responds elastically to stretching. For the motion of the interface we use Strain's semi-Lagrangian contouring method. The Stokes velocity is computed as a potential integral in a periodic box using Ewald summation, with the smooth part found as a Fourier series and the remaining part treated as a local correction.

Fast solvers for fluid membranes in 2D. **George Biros** (University of Pennsylvania, USA) IC/MT2812/014

Fluid membranes are area-preserving interfaces that resist inbending. They are common in biophysics as they model cell membranes, vesicles, and viral particles. In this talk we will discuss fast solvers for the time evolution of fluid membranes immersed in a Stokesian fluid. In particular we will discuss time-stepping, stability restrictions, and stiffness. The overall formulation is based on a spectral adaptive discretization and a boundary integral formulation for the Stokes operator.

IC/MP70/014: Automatic differentiation: applications and tools.

Organiser: Uwe Naumann (RWTH Aachen, Germany)
Co-organiser: Paul Hovland (Argonne National Laboratory, USA)

The ability to compute derivatives of outputs of numerical simulation programs with respect to a potentially very large number of parameters plays an increasingly important role in the attempt to make the transition from mere simulation of real-world processes to the highly desirable optimization of the numerical models. Adjoint models in particular are crucial prerequisites for the successful solution of the arising large-scale nonlinear optimization problems. Classical numerical differentiation may lack the desired accuracy. More importantly, the computational complexity of finite differences makes it simply inapplicable to large-scale problems. Hence, many man years have been invested into developing and maintaining such models manually.

Software tools for automatic differentiation (AD) are being developed with the aim to make the computation of derivatives robust, efficient, and potentially fully automatic. They have proved extremely useful in a wide range of applications. The state of the art in both the application of AD technology and the development of new AD tools is described in Bücker, Corliss, Hovland, Naumann, Norris: *Automatic Differentiation: Applications, Theory and Implementations*, LNCSE 50, Springer, 2006. Links to research groups and tool developers as well as descriptions of applications and an extensive bibliography on the subject can be found on the AD-community's Internet site www.autodiff.org.

This minisymposium consists of two sessions. Following a gentle introduction to the principles behind AD three presentations of applications set the stage for four talks about modern AD tools for Fortran and C/C++. The target audience comprises everybody who requires derivatives of mathematical models implemented as numerical simulation programs written in C/C++ or Fortran. Our aim is to make AD technology accessible to a wider range of potential users.

The OpenAD project: ADIC 2.0 and OpenAD/F. **Paul Hovland** (Argonne National Laboratory, USA), Boyana Norris (Argonne National Laboratory, USA), Jean Utke (Argonne National Laboratory, USA) IC/MT2535/014

We describe the OpenAD project, which includes two tools, ADIC 2.0 and OpenAD/F, for the automatic differentiation of ANSI C and Fortran 90, respectively. We introduce the tool architecture, which includes several shared components, including the xaif XML schema for representing the mathematically relevant aspects of a computation, the xaifBooster transformation engine, and the OpenAnalysis framework for compiler analyses. We discuss ongoing work on efficient second derivative (Hessian) computations and efficient derivative computations for MPI-parallelized applications. We highlight the use of the tools in several applications.

Adjoint-based quasi-Newton methods. **Andreas Griewank** (Humboldt-Universität zu Berlin, Germany) IC/MT2967/014

The cheap evaluation of Jacobian vector-products facilitated by the reverse mode of automatic differentiation opens up a new avenue of low rank updating. One resulting update formula combines the properties of heredity and least change stability, which can be shown to imply the attainment of the maximal convergence order achievable by secant methods.

Adjoint-enabled NAGWare *Fortran compiler.* **Jan Riehme** (University of Hertfordshire, UK), Uwe Naumann (RWTH Aachen, Germany) IC/MT3136/014

CompAD-II is the successor of a very successful collaboration between the University of Hertfordshire,Hatfield, UK and the Numerical Algorithm Group (NAG), Oxford, UK.

Whereas CompAD-I was focused on the first-time integration of forward mode Automatic Differentiation within an industrial strength compiler, the main goal of CompAD-II is to implement a robust adjoint mode in the NAGWare Fortran 95 compiler.

The user has to compile the top-level routine with the new `-ad` compiler switch. Than the compiler will do all necessary type changes for active variables automatically without further user interaction.

We will use a hybrid approach combining source transformation and overloading techniques that allows us a stepwise transition from an almost overloading based first prototype towards source transformation tool by replacing overloaded operators step by step with direct modifications on the compiler internal representation at compile time.

We will present the results of the first 10 months of the CompAD-II project and will give an outlook to the remaining duration of project (14 month).

ADiCape: AD for portable process systems models. **Monika Petera** (RWTH Aachen, Germany) IC/MT1156/014

CapeML is a platform independent XML-based language for describing models in process systems engineering. ADiCape is an XSLT-based differentiation tool for the automatic differentiation of model equations expressed in CapeML. The ADiCape tool currently employs the forward mode of AD in the computation of first and second order derivatives, including an interface for sparsity aware compression of Jacobian and Hessian matrices. Here we report on the design of ADiCape, including recent optimizations to account for the equation-based nature of CapeML "programs", as well as applications in large-scale process control engineering.

IC/MP70/014: Automatic differentiation: applications and tools. #2

Organiser: Uwe Naumann (RWTH Aachen, Germany)
Co-organiser: Paul Hovland (Argonne National Laboratory, USA)

(For abstract, see session #1 above.)

Introduction to automatic differentiation. **Uwe Naumann** (RWTH Aachen, Germany) IC/MT543/014

This introduction to Automatic Differentiation (AD) is to set the stage for the following talks. We will review the forward and reverse modes as well as point out issues in tool development and derivative code optimization. Our objective is that everybody in the audience will be familiar with the concepts of tangent-linear code (generated by forward mode AD), adjoint code (generated by reverse mode AD), and approaches to AD tool development based on source transformation or overloading.

Automatic differentiation for C and C++ codes: ADOL-C. **Andrea Walther** (TU Dresden, Germany) IC/MT1037/014

The AD-package ADOL-C uses operator-overloading for the Automatic Differentiation of C and C++ codes: Each double variable on the path from the independent variables to the dependents is replaced by a variable of the new type adouble introduced by ADOL-C. During the evaluation of the function to be differentiated the usage of the new data-type adouble causes the generation of an internal function representation called *tape*. Subsequently this internal representation is used to compute the desired derivative objects.

Several drivers provided by ADOL-C allow a very flexible choice of the mode and order of differentiation to be performed, including the computation of higher derivative tensors and sparsity structures. Furthermore, the Taylor coefficient vectors and their Jacobians with respect to the current state vector of solution curves defined by ordinary differential equations can be calculated. Note that ADOL-C can handle codes based on classes, templates and other C++-features. The derivative calculations involve a possibly substantial but always predictable amount of data that are accessed strictly sequentially. The much smaller randomly accessed memory can be precalculated using information on the tape.

The tape can be used to calculate derivatives for other arguments as long as the control flow of the program stays the same. Hence, the ideal situation is to generate the tapes once and reuse them for all derivative calculations. Then the effort of logging the whole function evaluation should be negligible.

The talk sketches the overloading strategy in more detail including the taping mechanism of the internal representation. Furthermore, recent developments, including checkpointing facilities, are presented. Finally, some examples illustrate applications of ADOL-C.

TAPENADE: a tool for automatic differentiation of programs. **Benjamin Dauvergne** (INRIA Rocquencourt, France) IC/MT2314/014

We present TAPENADE, a tool for Automatic Differentiation (AD) by program transformation. Given a Fortran77 or Fortran95 program that evaluates a function, TAPENADE can produce tangent programs that compute directional derivatives, and adjoint programs that compute gradients. Documentation of TAPENADE, together with access to the tool itself, are available on our web site http://www-sop.inria.fr/tropics. TAPENADE development started in 1999, and it has now a wide range of applications on industrial codes. We will show how the principles of AD are reflected in TAPENADE's differentiation model, and illustrate internal algorithms and results on some code examples.

Gradients are probably the most promising derivatives, as they are essential in optimization. Therefore, they receive a particular attention and development effort in TAPENADE. We would like to emphasize the static data-flow analysis techniques that make AD-generated adjoints perform comparably to good hand-written tangents or adjoints, at a cheaper development cost. In particular, the proeminent features of the tool are activity analysis, TBR analysis, and dead adjoint code elimination, all of them running interprocedurally. The reverse mode of TAPENADE is based on the so-called "Store-All" approach, combined with Checkpointing. We will show how TAPENADE can let the end-user refine from the default automatic checkpointing choices, and we will discuss some experimental heuristics that can refine these choices mechanically.

We shall show some successful applications of TAPENADE to large scale applications: gradient-based shape optimization in CFD, and variational data-assimilation in Earth sciences. We will conclude with a discussion on present limitations of the AD model and a description of future tool developments.

AD in meteorology. **Peter Korn** (Max-Planck-Institut für Meteorologie, Germany) IC/MT2758/014

The first part of this talk gives an overview of the applications of Automatic Differentiation (AD) in modeling the atmosphere and ocean circulation. The emphasis of the overview is placed on variational data assimilation methods. The mathematical basis for these methods is provided by the adjoint method of optimal control theory. The second part of the talk focuses on the challenge that is imposed by the presence of turbulence on AD based methods of adjoint flow control. We show results that indicate that turbulence closure via Lagrangian averaging provides a suitable framework for the control of three-dimensional turbulent flow.

IC/MP646/010: Lattice-Bolzmann methods for multiphase fluid and particle suspension flows.

Organiser: Omar al-Khayat (Simula Research Laboratory, Norway)
Co-organiser: Hans Petter Langtangen (Simula Research Laboratory, Norway)

Over the recent years, Lattice Boltzmann methods (LBM) have proven to be a viable alternative to traditional CFD in fluid flow simulations. Originating from Physics, LBMs have been successfully used in many cross-disciplinary fields of applied science. In many cases, the LBM approach has allowed relatively easy ways of simulating processes that are difficult or impossible to model by traditional CFD methods. In this minisymposium we will present various aspects of the LBM approach, including implementation, optimization, and its applicability for geoscientific problems, such as multiphase flow and depositional processes.

Simulations of dynamic properties of suspensions. **Dewei Qi** (Western Michigan University, USA) IC/MT3581/010

A review of spherical, non-spherical, rigid and flexible particle suspensions by using lattice Boltzmann simulations will be given. In particular, the method for flexible fiber suspensions is developed. The applications of the flexible fiber suspension in shearing, sedimenting and pressure driven flows will be presented. Effects of fiber flexibility on micro structure and rheological properties are studied and reported.

Lattice-Boltzmann model for dissolution phenomena. **Frederik Verhaeghe** (Katholieke Universiteit Leuven, Belgium) IC/MT1670/010

In this talk we present a lattice Boltzmann model for complex dissolution phenomena in three dimensions. We study the dissolution behaviour of a spherical particles in a cubic enclosure with and without double-diffusive natural convection. The results are compared with dissolution experiments conducted with a confocal scanning laser microscope with heat stage.

Hybrid parallelization techniques for lattice-Boltzmann free surface flows. **Ulrich Rüde** (Universität Erlangen–Nürnberg, Germany) IC/MT5050/010

This talk will present an algorithm to perform adaptive free surface simulations with the lattice Boltzmann method (LBM) on machines with shared and distributed memory architectures. Performance results for different test cases and architectures will be given. The algorithm for parallelization yields a high performance, and can be combined with the adaptive LBM simulations. Moreover, the effects of the adaptive simulation on the parallel performance will be evaluated.

This is a joint work with Nils Thuerey.

IC/MP285/010: Mathematical algorithms, frameworks, and scientific applications on large-scale parallel machines.

Organiser: Xiaoye Li (Lawrence Berkeley National Laboratory, USA)
Co-organiser: Osni Marques (Lawrence Berkeley National Laboratory, USA)

The development of high performance simulation codes is a demanding process, due to the complexity of the phenomena to be simulated as well as the growing sophistication of computer architectures. The success of such efforts requires close collaboration of domain scientists, applied mathematicians and computer scientists in the process of developing models, implementing numerical algorithms, and performing code optimization to achieve optimal use of the computational resources.

The purpose of this minisymposium is twofold. Firstly, it focuses on a set of cutting edge mathematical tools, portable software libraries, and friendly frameworks being developed and used to tackle scientific computing applications. The availability of such advanced tools has enabled more complex physical phenomena to be addressed and as a result contributed to the growth of the computational sciences community. Secondly, the minisymposium includes presentations on a set of challenging applications, such as electronic structure calculations, modeling of incompressible flow, and electromagnetic problems. These applications require significant computing resources but have also fostered the development of novel mathematical tools and revealed new opportunities in algorithm research.

Evaluation of the AMLS method for sparse eigenvalue problems. **Xiaoye Li** (Lawrence Berkeley National Laboratory, USA) IC/MT1149/010

We describe an efficient implementation and present a performance study of an algebraic multilevel sub-structuring (AMLS) method for sparse eigenvalue problems. We assess the time and memory requirements associated with the key steps of the algorithm, and compare it with the shift-and-invert Lanczos algorithm in computational cost. Our eigenvalue problems come from two very different application areas: the accelerator cavity design and the normal mode vibrational analysis of the polyethylene particles. We show that the AMLS method, when implemented carefully, is very competitive with the traditional method in broad application areas, especially when large numbers of eigenvalues are sought.

This is joint work with Weiguo Gao, Chao Yang, and Zhaojun Bai.

The use of hybrid techniques at CERFACS for the solution of large-scale problems on parallel machines. **Iain Duff** (Rutherford Laboratory & CERFACS, UK), Serge Gratton (CERFACS, France), Xavier Vasseur (CERFACS, France) IC/MT2087/010

In this talk we will review some recent developments on the combined use of direct and iterative methods for solving very large linear systems of equations, such as those arising in the solution of large 3D PDE's.

We first examine the size of the largest problems that can be solved by current direct methods in 2007. We then discuss some of the algorithmic developments undertaken by the developers of these methods to solve larger problems. Current areas of investigation include the use of out-of-core techniques, and the parallelization of the symbolic factorization phase. An obvious alternative to direct methods are iterative methods. However, it is well known that they encounter difficulties for large ill-conditioned or ill-scaled problems. In these cases, iterative methods may exhibit poor convergence if not adequately preconditioned. We review how these two types of methods can be combined to solve very large and sparse linear systems. A successful combination that will be specially considered is the use of a Krylov method preconditioned by some technique involving a direct method.

In this talk, we will focus on two main applications. For the first, an approximate factorisation of the matrix is performed using static pivoting strategies. We show how the solution of symmetric indefinite problems can be refined by a Krylov method to yield a backward stable solution of the original problem. Secondly, we consider the numerical simulation of seismic wave propagation in three dimensions. This requires a robust and fast solution of the Helmholtz equation. A multigrid method used as a preconditioner for a Krylov method is investigated. We will examine the effect of incorporating the direct solver inside the multigrid framework and its impact on the preconditioner and illustrate the performance of this approach on our parallel machines at CERFACS.

Adaptive numerical components for PDE-based simulations. **Boyana Norris** (Argonne National Laboratory, USA), Lois McInnes (Argonne National Laboratory, USA), Sanjukta Bhowmick (Argonne National Lab. & Columbia Univ., USA), Dinesh Kaushik (Argonne National Laboratory, USA) IC/MT2567/010

Numerical simulations based on nonlinear PDE solution using Newton-based methods require the solution of large, sparse linear systems of equations at each nonlinear iteration. Typically in large-scale parallel simulations such linear systems are solved using iterative preconditioned Krylov methods. In many cases, especially in time-dependent problems, the linear system characteristics can change throughout the stimulation, potentially leading to varying times for solving the linear systems in different nonlinear iterations. We present an approach to characterizing the nonlinear and linear system solution and using the resulting application performance information to dynamically select linear solver methods with the goal of reducing the total time to solution. We discuss the effect of these adaptive heuristics on a number of applications, including fluid dynamics and radiation transport simulation codes. We also present a general component infrastructure for the support of dynamic algorithm selection and adaptation in applications involving the solution of nonlinear PDEs.

EigAdept: an expert eigensolver toolbox. **Osni Marques** (Lawrence Berkeley National Laboratory, USA), Xiaoye Li (Lawrence Berkeley National Laboratory, USA) IC/MT1779/010

The computation of eigenvalues and eigenvectors is an important and often time-consuming phase in a large range of computer simulations. Recent efforts in the development of libraries that implement eigenvalue solvers have provided domain scientists with robust algorithms, without the need for domain scientists to spend much time in programming. Yet, given the variety of numerical algorithms that are available to a practitioner, the choice of the *optimal* algorithm for increasingly sophisticated and larger applications is a daunting task. In this presentation we discuss a methodology and a software toolbox that aims at guiding a practitioner through the maze of various eigenvalue solvers with different configurations, and at determining the more appropriate solver based on the type of the application the properties of the associated matrices.

IC/MP285/010: Mathematical algorithms, frameworks, and scientific applications on large-scale parallel machines. #2

Organiser: Xiaoye Li (Lawrence Berkeley National Laboratory, USA)
Co-organiser: Osni Marques (Lawrence Berkeley National Laboratory, USA)

(For abstract, see session #1 above.)

Implicit methods for low Reynolds-number free-surface flows. **José Cuminato** (Universidade de São Paulo, Brazil) IC/MT788/010

One the most widely used methods in computational fluid dynamics for solving satisfactorily free surface flow problems, governed by the Navier-Stokes equations, is the MAC method [F.H. Harlow and J.E. Welch, Physics of Fluids, 8 (1965) 2182-2189]. Based on the MAC method, many techniques have been developed for solving problems in computational rheology. Generally, these methods use an explicit formulation, as GENSMAC (GENeralized Simplified Marker-And-Cell) method [M.F. Tomé and S. McKee, J. Comput. Phys., 110 (1994) 171-186]. The explicit time discretization introduces the parabolic stability restriction, making, for some applications, the time step very small when the Reynolds number is much smaller than 1. This fact justifies the need for methods with better stability properties like implicit schemes. In this work, we present a stable semi-implicit formulation for the numerical solution of transient, Newtonian and incompressible flows based on splitting the original problem into successive subproblems cheaper to solve. This formulation is known as fractional step or projection method and aim at calculating the velocity and pressure fields separately. The boundary conditions (free surface and rigid) are discretized implicitly to preserve the stability of the semi-implicit method. The numerical results demonstrate that the present technique eliminates the parabolic stability restriction required by the original explicit GENSMAC method, and also found in segregated semi-implicit methods with time-lagged boundary conditions. For low Reynolds number flows, the method is robust and very efficient when compared to the original GENSMAC method.

Parallel performance issues for multiphysics adaptive mesh-refinement algorithms. **John Bell** (Lawrence Berkeley National Laboratory, USA) IC/MT1481/010

Adaptive Mesh Refinement (AMR) is an effective tool for the solution of partial differential equations often requiring far fewer computational resources as compared to equivalently resolved non-adaptive calculations. Hierarchical approaches AMR algorithms, originally developed for gas dynamics, are now used in a number of multiphysics applications. The added algorithmic complexity of AMR algorithms combined with the requirements of multiphysics applications makes parallelization of these types of algorithms a challenging topic. Key issues in developing efficient parallel implementations include load balancing, data distribution, non-numerical metadata manipulations and linear solvers. In this talk, we will discuss each of these issues in the context of several applications drawn from combustion, astrophysics and subsurface flow. For each issue we will characterize the difficulty and describe approaches to improving performance. Finally, we will discuss the impact of these algorithmic improvements on overall scaling behavior.

Derivative-free optimization methods for surface structure determination of nano-systems. **Juan Meza** (Lawrence Berkeley National Laboratory, USA) IC/MT1267/010

Many properties of nanostructures depend on the atomic configuration at the surface. One common technique used for determining this surface structure is based on the low energy electron diffraction (LEED) method, which uses a sophisticated physics model to compare experimental results with spectra computed via a computer simulation. While this approach is highly effective, the computational cost of the simulations can be prohibitive for large systems. In this work, we propose the use of generalized pattern search methods for determining the surface structure of nanosystems. The generalized pattern search method handles both discrete and continuous variables, which allows the simultaneous optimization of the atomic coordinates as well as the chemical identity. We also propose using a simplified physics surrogate in place of the full fidelity physics model. We will present some numerical results based on this simplified physics surrogate within a pattern search method.

New eigensolvers for scalable nano-science simulations. **Andrew Canning** (Lawrence Berkeley National Laboratory, USA) IC/MT2053/010

We present results for new iterative eigensolvers based on conjugate gradients and Jacobi-Davidson in the context of semi-empirical plane wave electronic structure calculations. These new methods give significant speedup over existing conjugate gradient methods used in electronic structure calculations. The new methods will be demonstrated for CdSe quantum dots as well as quantum wires constructed from layers of InP and InAs. These systems are studied in the context of a semi-empirical potential where we typically solve for a few states around the gap allowing us to study large scale nanaosytems. The parallelization of this approach will also be discussed as well as scaling results to large processor counts. Work carried out in collaboration with Osni Marques, Christof Voemel, Lin-Wang Wang, Stanimire Tomov, Julien Langou and Jack Dongarra.

IC/MP355/010: An outlook on scientific software libraries.

Organiser: Osni Marques (Lawrence Berkeley National Laboratory, USA)

The development and implementation of simulation codes on current computer platforms is often a demanding and costly process, due to the complexity of the phenomena to be simulated but also to the proliferation and evolution of computer architectures. The success of such efforts is dictated by the time required to achieve a functional prototype code of the application, and then an optimized production version of the code in order to achieve an optimal usage of the available computational resources. Today, high quality scientific software libraries are widely used in simulation codes.

Despite the recognized value of such libraries, from reducing time to solution to achieving performance, their future is unclear. Demand for more sophisticated simulations requires programmers to be more productive. This pushes toward larger, more integrated and more capable, environments or packages, but with significant disagreement in the scientific community as to the form these should take. At the same time, funding support even for our present-day capabilities has become an acute problem. Funding agencies usually do not fund software support, if they even fund its development. We expect important libraries to be readily available and delivering high performance on all architectures, but computer vendors may not have the resources to do the necessary optimization, especially as packages grow in size and capability. The computation science community is reluctant to pay for libraries, so commercializing software development and support is still largely a cottage industry.

In this minisymposium we propose to bring together different perspectives about these conflicting expectations from users and vendors. We also propose to discuss new technological trends, and most importantly, whether the concept of scientific libraries is obsolete.

Quality assurance: the way forward. **Tim Hopkins** (University of Kent, UK) IC/MT1289/010

I don't believe that software libraries per se are doomed – their usage and interfaces may well change but library codes will still form the core of numerical simulations for the foreseeable future. What does need to change is the way in which library software is deemed fit for purpose; my contact with scientific software as editor for ACM CALGO has convinced me that while the standard of numerical algorithms and techniques has continued to improve the associated software products rarely do the algorithm justice. I would like to see a system whereby software can give a quality rating. This could be partially based on software metrics which would be used to provide indications of code quality, levels of testing, maintenance levels, etc. but would also include peer reviews/comments. It would seem sensible to piggy back such a system on to some form of "son-of-netlib" in the form of a numerical SourceForge; in this way groups of interested users/developers would be able to maintain and improve the software. (This is another area where even good projects (for example, LAPACK and ScaLAPACK) falter – updates/bug fixes etc are very slow at reaching the released packages.)

A forecast of Open Source *and commercial futures for scientific software.* **John Nash** (Université d'Ottawa, Canada) IC/MT1263/010

This talk will look at the infrastructure for scientific software, that is, the procedures, tools, functions and basic knowledge that are used to build scientific software. Examples include compilers, function and subroutine libraries, packages that are used to build other packages, and the collection of papers, reports, and correspondence that collectively provide the background to such work. There appears to be anecdotal evidence – indeed I have some personal experience – that the grant and investment support for such infrastructure has declined in the last two decades. Yet support is needed as new architectures and technologies for scientific computing become available such as inexpensive clusters or grids, particularly those with heterogeneous nodes, and quantum computers. Also, new domains of application, such as some areas of biotechnology and environmental modelling, will require new adaptations or streamlining. The author will attempt to provide some possible futures for scientific software, in particular with a view of both open source projects and commercial ventures.

Do commercial scientific software libraries have a future?. **Ian Reid** (NAG Ltd, UK) IC/MT1848/010

We explore the pros and cons of using commercial scientific software libraries versus open source/DIY. We look at how the marketplace for such software has changed over the last 30 years, how it is used today, and the prospects for the future given the (r)evolution of the hardware.

ACTS: a collection of robust and high-performance software tools. **Osni Marques** (Lawrence Berkeley National Laboratory, USA) IC/MT1780/010

The development of efficient simulation codes is an expensive process that often requires specialized support and information about the available computational resources and software tools. The development effort is usually augmented by the complexity of the phenomena that can be addressed through computers simulations, along with the increase and evolution of computing resources. The US Department of Energy (DOE) Advanced Computational Software (ACTS) Collection comprises a set of DOE-developed software tools, sometimes in collaboration with other funding agencies, and that aim at simplifying the development of computational sciences applications. The talk will describe the functionalities that the tools provide, categories of problems that the tools can solve, availability, portability, and a number of applications that have benefited from the tools, and issues related to long-term support and maintenance.

IC/MP81/010: Uncertainty quantification in computational science and engineering.

Organiser: Fabio Nobile (Politecnico di Milano, Italy)
Co-organiser: Raul Tempone (Florida State University, USA)

Numerical simulations are used every day more as tools to predict the behavior of complex physical systems. Thanks to the fast growing computer power and improved discretization techniques, we are now able to solve more complex systems of partial differential equations in reasonable time.

Yet, many engineering applications, such as groundwater flows, environmental problems, composite materials, reactive flows, just to name a few, are affected by a relative large amount of uncertainty. For instance, the mathematical model used to describe these applications might present uncertainty in the geometry, boundary or initial conditions, model parameters, etc.

Computational Engineering is now facing a new challenge on how to properly incorporate those sources of uncertainty as well as propagate them to the output of numerical simulations.

The Mini-symposium aims at showcasing recent deterministic and probabilistic techniques proposed for Uncertainty Quantification, including Stochastic Galerking, Stochastic Collocation, Stochastic perturbation, Monte Carlo techniques, sensitivity analysis, worst-case scenario, fuzzy sets, etc.

Sparse wavelet methods for operator equations with stochastic data. **Christoph Schwab** (ETH Zürich, Switzerland) IC/MT369/010

Let $A: V \to V'$ be a strongly elliptic operator on a d-dimensional manifold D. An operator equation $Au = f$ with stochastic data f is considered. The goal of the computation is the mean field and higher moments $\mathcal{M}^1 u \in V$, $\mathcal{M}^2 u \in V \otimes V$, $\ldots, \mathcal{M}^k u \in V \otimes \cdots \otimes V$ of the solution.

We discretize the mean field problem using a FEM with hierarchical basis and N degrees of freedom. We present a Monte-Carlo algorithm and a deterministic algorithm for the approximation of the moment $\mathcal{M}^k u$ for $k \geq 1$.

The key tool in both algorithms is a *sparse tensor product* space for the approximation of $\mathcal{M}^k u$ with $O\left(N(\log N)^{k-1}\right)$ degrees of freedom, instead of N^k degrees of freedom for the full tensor product FEM space.

A sparse Monte-Carlo FEM with M samples (i.e., deterministic solves) is proved to yield approximations to $\mathcal{M}^k u$ with a work of $O(MN(\log N)^{k-1})$ operations. The solutions are shown to converge with the optimal rates with respect to the number N of Finite Element degrees of freedom and the number M of MC samples.

The deterministic FEM is based on hypoelliptic equations for $\mathcal{M}^k u$ in $D^k \subset R^{kd}$. Their Galerkin approximation using sparse tensor products of the FE spaces in D allows approximation of $\mathcal{M}^k u$ with $O\left(N(\log N)^{k-1}\right)$ degrees of freedom converging at an optimal rate (up to logs). For nonlocal operators wavelet compression of the operators is used.

The linear systems are solved iteratively with multilevel preconditioning. This yields an approximation for $\mathcal{M}^k u$ with at most $O\left(N(\log N)^{k+1}\right)$ operations.

Applications of the method include $O(N)$ algorithms for the second order statistics of solutions to elliptic problems in domains with random boundary.

This is joint work with Tobias von Petersdorff (Univ. Maryland, College Park).

Stochastic collocation methods for elliptic PDEs with random input data. **Raul Tempone** (Florida State University, USA), Fabio Nobile (Politecnico di Milano, Italy), Clayton Webster (Florida State University, USA) IC/MT3389/010

We present a stochastic-collocation method to solve partial differential equations with random coefficients and forcing terms (input data of the model). The input data are assumed to depend on a finite number of random variables. The method consists in a Galerkin approximation in space and a collocation in the zeros of suitable tensor product orthogonal polynomials (Gauss points) in the probability space and naturally leads to the solution of uncoupled deterministic problems as in the Monte Carlo approach.

We will present collocation techniques based on full anisotropic tensor product grids as well as isotropic or anisotropic sparse grids based on the Smolyak construction. The last approach is particularly attractive in the case of input data obtained as truncated expansions of random fields, since the anisotropy can be tuned on the decay properties of the expansion We will present *a priori* and *a posteriori* ways to chose the anisotropy of the sparse grid which are extremely effective in some situations.

We will also present rigorous convergence results in all cases as well as numerical examples where we compare the different approaches with the more traditional Monte Carlo technique. In particular, the sparse grid approach, with a properly chosen anisotropy seems to be very efficient and superior to all the others also when a moderately large number of input random variables is considered.

[1] Babuška, I., Nobile, F. and Tempone, R.; A stochastic collocation method for elliptic partial differential equations with random input data. MOX Report No. 71, 2005, accepted for publication on SIAM J. Numer. Anal.

[2] Nobile, F., Tempone, R. and Webster, C; A sparse grid stochastic collocation method for elliptic partial differential equations with random input data. MOX Report 85, 2006, submitted.

[3] Nobile, F., Tempone, R. and Webster, C; An anisotropic sparse grid stochastic collocation method for elliptic partial differential equations with random input data. in preparation.

A mapping approach for the numerical solution of PDEs on stochastic domains. **Davide Fransos** (Politecnico di Torino, Italy), Claudio Canuto (Politecnico di Torino, Italy) IC/MT2408/010

The present work focuses on the numerical solution of stochastic partial differential equations of elliptic type, posed in a domain whose boundary is described by random variables. Possible solution approaches are based on the Fictitious Domain method [2] and on stochastic mappings [3]. Following the latter, a Polynomial Chaos (PC) expansion expresses the stochastic parametrization of the boundary. Then, it is possible to extend the parametrization inside the domain, i.e., to map the random domain onto a fixed one: the PDE of interest is converted into a new one, posed in a non-random domain but with random coefficients and data (recent results for such equations can be found in [1]). Discretization is accomplished by h-type finite elements in the deterministic variables and orthogonal polynomial projection in the stochastic variables. In the case of a small number of PC variables, the discrete variational formulation features a Galerkin projection onto complete tensor-product spaces of stochastic variables and tensor-product numerical integration in these variables. The resulting scheme is equivalent to a collocation scheme, i.e., to a non-intrusive treatment of stochasticity. This yields a very efficient method, e.g. in comparison with Monte Carlo methods. When the number of PC variables becomes larger than a certain value, the need for "sparse" quadratures arises. The latter case is considered herein.

[1] Ivo Babuška, Fabio Nobile, and Raúl Tempone. A stochastic collocation method for elliptic partial differential equations with random input data. Technical Report 71, MOX, Politecnico di Milano, 2005.

[2] Claudio Canuto and Tomáš Kozubek. A fictitious domain approach to the numerical solution of pdes in stochastic domains. Technical Report 12, Politecnico di Torino, Dip. di Matematica, 2006.

[3] Dongbin Xiu and Daniel M. Tartakovsky. Numerical methods for differential equations in random domains. *SIAM J. Sci. Comput.*, 28(3):1167–1185 (electronic), 2006.

Error estimation and adaptive computation for elliptic problems with randomly perturbed coefficients and data. **Axel Målqvist** (UC San Diego, USA), Donald Estep (Colorado State University, USA), Simon Tavener (Colorado State University, USA) IC/MT1805/010

Uncertainty in data and coefficients has important consequences for the solutions of otherwise deterministic elliptic problems. Developing efficient methods for understanding the effects of uncertainty is a significant problem in many practical applications. Such uncertainty might arise for example from error in experiments used to measure parameter values, or as a result of coupling to other physical systems. In such settings, the uncertainty is best described as random in nature. This leads to the problem of describing the response in a quantity of interest computed from the solution resulting from the stochastic variations in parameters and data. This is a difficult problem for a number of reasons for example computing a large number of samples is usually prohibitively expensive and numerical error typically varies as parameters and data vary.

We develop and analyze an efficient numerical method for computing the response of a quantity of interest derived from the solution of an elliptic problem with randomly perturbed coefficients and data. We use a variational analysis based on the adjoint operator for problems with uncertainty in the data and boundary conditions. For problems with uncertainty in the diffusion coefficient, we construct a piecewise constant approximation to the random perturbation then use domain decomposition to decompose the problem into sub-problems on which the diffusion coefficient is constant. To compute local solutions of the sub-problems we truncate the infinite series for the matrix inverse. Finally, we derive *a posteriori* error estimates that take into account all the sources of error and derive a new adaptive algorithm that provides a quantitative way to distribute computational resources.

IC/MP412/010: Uncertainty quantification in computational science and engineering, III.

Organiser: Fabio Nobile (Politecnico di Milano, Italy)
Co-organiser: Raul Tempone (Florida State University, USA)

Numerical simulations are used every day more as tools to predict the behavior of complex physical systems. Thanks to the fast growing computer power and improved discretization techniques, we are now able to solve more complex systems of partial differential equations in reasonable time.

Yet, many engineering applications, such as groundwater flows, environmental problems, composite materials, reactive flows, just to name a few, are affected by a relative large amount of uncertainty. For instance, the mathematical model used to describe these applications might present uncertainty in the geometry, boundary or initial conditions, model parameters, etc.

Computational Engineering is now facing a new challenge on how to properly incorporate those sources of uncertainty as well as propagate them to the output of numerical simulations.

This mini-symposium aims at showcasing recent deterministic and probabilistic techniques proposed for Uncertainty Quantification, including Stochastic Galerking, Stochastic Collocation, Stochastic perturbation, Monte Carlo techniques, sensitivity analysis, worst-case scenario, fuzzy sets, etc.

Uncertainty quantification using probability logic and its application to robust predictive modelling of systems. **James Beck** (California Institute of Technology, USA) IC/MT3591/010

Probability can be viewed as a multi-valued logic that extends Boolean propositional logic to the case of incomplete information. The key idea is that the probability $P(b|c)$ of a statement b, given the information in statement c, is a measure of how plausible b is based on c. Boolean logic deals with the special case of complete information where the truth or falsity of b is known from c. This interpretation is consistent with the Bayesian one that probability repesents a degree of belief in a statement. Kolomogorov's axioms for probability, which are neutral with respect to interpretation of the probability measure, are a special case where the statements refer to sets. Probability logic provides a rigorous unifying framework for treating modeling uncertainty, along with excitation uncertainty, when using models to predict the response of a system. This paper gives an overview of its foundations and its application to quantifying uncertainty for predictive modeling of systems. The key concept of a Bayesian model class will be described, which is a set of possible probabilistic predictive models for a system together with a probability distribution over this set to quantify the plausibility of each model. Based purely on the probability axioms, a Bayesian model class leads to both prior (initial) and posterior (updated using test data) robust predictive models. Since there is always uncertainty in choosing a model class to represent a system, one can also choose a set of candidate model classes. The probability axioms then lead naturally to prior and posterior hyper-robust predictive models. The challenge in implementations is that integrals over high-dimensional parameter spaces are usually involved that cannot be evaluated in a straight-forward way. Useful computational tools are asymptotic approximations and stochastic simulation based on Markov Chain Monte Carlo methods. Illustrative examples will be presented based on the work of the author and his colleagues.

Tools for model validation based on incomplete data. **Helmut Pradlwarter** (Universität Innsbruck, Austria) IC/MT2397/010

Data to establish probability distributions to describe the variability of some physical properties is quite often very scarse and measurements to increase the sample size are expensive. Under such circumstances, there is little credibility for any *a priori* selected type of distribution. Moreover, the variability of possible distributions due to the lack of sufficient data, is generally ignored by using standard parameter estimation procedures such as the methods based on moments or the Maximum Likelihood. In this paper the use of kernel densities is proposed, where the dispersion of the kernel is a quantitative function of the number of available data points and the required confidence level. Hence, the tails of the distribution, which might be decisive for the reliability assessmnet, will be established as a function of the available number of data point and a reasonable confidence that the probability in the tails will not be higher as assumed. Kernel densities are especially suitable to assign joint probability distributions to data with several components, where the observed correlation among the components must be respected which is usually very cumbersome using traditional approaches. The proposed approach will be demonstrated by applying it for insuffient data provided in the "Model validation problem: Static frame problem", proposed in [1], where a bivariate probability distribution is needed to assess the reliability by a probabilistic approach. Once the joint distribution has been established, an appropriate physical model to describe the variability of a random field, which is in

agreement with the joint distribution, is discussed. The problem will be solved by using a Monte Carlo based optimization procedure.

[1] I. Babuska, F. Nobile, and R Tempone. Model validation challenge problem: Static frame problem. In *Sandia, Validation Workshop*. Sandia, http://www.esc.sandia.gov/VCMwebsite/vcmhome.html, Nov. 7, 2005.

Dynamic assessment of uncertain mechanical designs based on the fuzzy finite-element method. **Dirk Vandepitte** (Katholieke Universiteit Leuven, Belgium), David Moens (Katholieke Universiteit Leuven, Belgium) IC/MT2455/010

The continuous exponential growth of computational capabilities of modern computers clearly has an impact on the use of the numerical simulation techniques like the finite element (FE) method for engineering purposes. On the one hand, this evolution enables the use of very detailed and hence large FE models. Simultaneously, this evolution has paved the way for a number of computationally intensive analysis techniques derived from the classical FE technique (non-linear analysis, multiphysics...). Especially in the context of numerical design procedures, non-deterministic FE analysis has become a very important issue in the search for valuable utilisation of the available computational resources, as it provides in a cheap and fast tool to assess a new design at a very early stage in its development. This work focuses on the use of the fuzzy finite element method for dynamic design assessment of uncertain mechanical structures through a non-deterministic numerical analysis. The first part consists of a general theoretical discussion on the use of the fuzzy concept in finite element analysis. Next, an overview of recent implementation strategies of the fuzzy finite element code is presented, focusing more specifically on the dynamic behaviour of the design (eigenfrequencies, dynamic responses and acoustic radiation). In order to indicate the added value of the fuzzy finite element method in design, the possible application of the method in a typical product design process is discussed. Finally, the applicability is illustrated through a number of industrially sized design problems.

Random-matrix theory for stochastic structural dynamics. **Sondipon Adhikari** (University of Bristol, UK) IC/MT3523/010

Uncertainties need to be taken into account for credible results from high fidelity, physics and engineering-based numerical simulations. As a result, the quantification and propagation of uncertainties play a crucial role in today's predictive engineering science. Uncertainties can be broadly divided into *parametric uncertainty* (inherent variability/data uncertainty) and *nonparametric uncertainty* (lack of knowledge/model uncertainty). Within the past three decades the deterministic finite element method has been generalized to consider parametric uncertainties in a systematic manner by means of the Stochastic Finite Element Method (SFEM). In the context structural dynamics, using SFEM one usually obtains the random mass, stiffness and damping matrices. More recently a systematic approach to model nonparametric uncertainty is proposed. Using this method one can obtain the probability density function of the system matrices. Therefore, both parametric and nonparametric uncertainty modelling lead to matrix variate distributions describing the system matrices of a linear dynamic system. In this paper it is first proved that both parametric and non-parametric uncertainty can be modelled using a unified matrix variate distribution (similar to a noncentral Wishart distribution). Parametric and nonparametric uncertainty models can be identified as special cases of this general distribution. Once the random system matrices are 'known' via this distribution, using the random matrix theory exact analytical methods have been proposed for the solution of a set of *random algebraic equations* ($\mathbf{K}\mathbf{y} = \mathbf{f}$) and the *random eigenvalue problem* ($\mathbf{K}\phi_j = \lambda_j \mathbf{M}\phi_j$).

IC/MP81/010: Uncertainty quantification in computational science and engineering. #2

Organiser: Fabio Nobile (Politecnico di Milano, Italy)
Co-organiser: Raul Tempone (Florida State University, USA)

(For abstract, see session #1 above.)

Polynomial-chaos expansion of a particle-mesh method for uncertainty quantification in vortical flow. **Olivier Le Maître** (Université de Evry, France), Omar Knio (Johns Hopkins University, USA) IC/MT2263/010

We present a new mesh-particle scheme for uncertainty propagation in the incompressible 2D Navier-Stokes equations in the Boussinesq limit. The scheme incorporates a polynomial chaos (PC) expansion of the flow variables into a Lagrangian particle approximation of the governing equations. The scheme relies on a single set of Lagrangian particles which are convected by the mean flow velocity, while PC representations of their strengths (circulation and temperature) are updated to account for the uncertainty in diffusive and convective effects. An integral approximation of the stochastic coupling terms is derived following the framework of the deterministic particle strength exchange method. This integral approximation yields an algorithm which is stable (even for infinite Péclet numbers) and conservative at the discrete level.

Thanks to the usage of a unique set of particles for all the stochastic modes, improved algorithms devised for the deterministic particle methods can be readily implemented, including mesh-particle methods and adaptive remeshing techniques. These result in a method that combines the advantages of the particles discretization with the efficiency of PC expansions.

Numerical examples are presented which demonstrate the effectiveness of the method to diffusion or convection dominated problems involving significant uncertainty levels, a large number of particles, and high-order PC expansions.

Anisotropic sparse grid stochastic collocation methods for nonlinear partial differential equations with random input data. **Clayton Webster** (Florida State University, USA), Raul Tempone (Florida State University, USA), Fabio Nobile (Politecnico di Milano, Italy) IC/MT3643/010

This work analyzes an anisotropic sparse grid stochastic collocation method for solving several nonlinear partial differential equations with random coefficients and forcing terms (input data of the model). Here, we especially address the situation where the input data are assumed to depend on a moderately large number of random variables, where in general the *curse of dimensionality* is encountered. The Sparse Grid Stochastic Collocation method we utilize was first proposed and analyzed in [Nobile-Tempone-Webster, Technical report #85, MOX, Dipartimento di Matematica, 2006] and extending to anisotropic sparse grids in [Nobile-Tempone-Webster, In preparation]. These approaches consist of a Galerkin approximation in space and a collocation, in probability space, at the zeros of sparse tensor product spaces uti-

lizing either Clenshaw-Curtis or Gaussian interpolants. As a consequence of the collocation approach our techniques naturally lead to the solution of uncoupled deterministic problems as in the Monte Carlo method.

We provide a rigorous convergence analysis and demonstrate exponential convergence of the "probability error" with respect of the number of Gaussian points in each direction in the probability space, under some regularity assumptions on the random input data. However, if the number of random variables is large, the construction of the full tensor product spaces becomes infeasible, since the dimension of the approximating space grows exponentially fast with the number of random variables.

In such cases, this work utilizes anisotropic sparse tensor product spaces constructed from the Smolyak algorithm utilizing suitable abscissas. We also provide a rigorous convergence analysis of the fully discrete problem and demonstrates: (sub)-exponential convergence of the "probability error" in the asymptotic regime and algebraic convergence of the "probability error" in the pre-asymptotic regime, with respect to the total number of collocation points. Numerical examples exemplify the theoretical results and are used to compare this approach with several others, including standard Monte Carlo. In particular, for moderately large dimensional problems, the sparse grid approach, with properly chosen anisotropy, seems to be very efficient and superior to all examined methods.

Multigrid-based preconditioners for stochastic Galerkin formulation of the mixed steady-state diffusion problem. **Catherine Powell** (University of Manchester, UK) IC/MT4555/010

Fluid flow in porous media is often modelled under the assumption that the conductivity coefficients are known at every spatial location. However, simulations based on such oversimplifications cannot provide quantification of probabilities of unfavourable events. Stochastic Finite Element Methods (SFEMs) provide a framework for incorporating statistical information about spatial variability in the conductivity coefficients into computer simulations in such a way that comprehensive probabilistic information about the fluid velocity and pressure is obtained. Specifically, the conductivity coefficients and solution variables are represented as random fields.

SFEMs give rise to very large systems of linear equations and consequently have suffered from bad press. We report on fast, robust linear algebra techniques and preconditioning schemes based on multigrid methods, for solving the stochastic Galerkin formulation of the Darcy flow problem (the steady-state diffusion problem in mixed form) which leads to systems of saddle-point type. Note that we do not solve the primal formulation of this standard elliptic problem. We consider both the (easier) case where doubly orthogonal stochastic basis functions are applied leading to a large number of small deterministic solves and the more challenging case where one large coupled system has to be solved, either due to the choice of a standard orthonormal stochastic basis or due to the presence of a stochastically non-linear random field coefficient. We present some comparisons with the traditional Monte Carlo approach on test problems and show numerical results produced with the mixed SFEM for a realistic flow problem.

Part of this work was done in collaboration with Elisabeth Ullmann and Oliver Ernst at TU Bergakademie Freiberg and David Silvester at the University of Manchester.

Stochastic Krylov-subspace methods for flow in random porous media. **Hector Klie** (University of Texas at Austin, USA), Mary Wheeler (University of Texas at Austin, USA), Adolfo Rodriguez (University of Texas at Austin, USA) IC/MT1490/010

The present work establishes a comparative analysis of different Krylov-based methods for assessing uncertainty in porous media flow. We distinguish two main approaches: (1) stochastic reduced basis methods, and (2) stochastic perturbation methods. The former relies on the construction of an orthogonal basis from which projectors may be realized to perform the uncertainty analysis on a lower-dimensional space. These projection methods may be either Krylov-based (namely, SRBM), as proposed by P.B. Nair, A.J. Keane and other collaborators, or POD-based, as proposed by some other authors. Both of these two methods have close connections with model reduction techniques developed in optimal control theory.

Stochastic perturbation approaches are based on the idea of expressing input and corresponding outputs in terms of stochastic and perturbative polynomial expansions. By grouping terms and moments of the same order, the original stochastic equation is replaced by successive (and parallel) solutions of a set of deterministic equations. The contributions of these solutions are gathered to reconstruct the solution and different stochastic moments associated with the phenomena response. Among these approaches we highlight the Krylov–Karhenun–Loeve moment equation (KKLME) approach for the solution of stochastic PDEs arising in large-scale porous media flow applications. The use of Krylov methods here focuses on the treatment of systems with multiple right-hand sides with block seeded deflation methods.

We provide a set of numerical experiments illustrating the capabilities of SRBM and KKLME on different permeability field distributions for one- and two-phase flow formulations.

IC/MP103/010: Uncertainty quantification in computational science and engineering, II.

Organiser: Fabio Nobile (Politecnico di Milano, Italy)
Co-organiser: Raul Tempone (Florida State University, USA)

Numerical simulations are used every day more as tools to predict the behavior of complex physical systems. Thanks to the fast growing computer power and improved discretization techniques, we are now able to solve more complex systems of partial differential equations in reasonable time.

Yet, many engineering applications, such as groundwater flows, environmental problems, composite materials, reactive flows, just to name a few, are affected by a relative large amount of uncertainty. For instance, the mathematical model used to describe these applications might present uncertainty in the geometry, boundary or initial conditions, model parameters, etc.

Computational Engineering is now facing a new challenge on how to properly incorporate those sources of uncertainty as well as propagate them to the output of numerical simulations.

The mini-symposium aims at show-casing recent deterministic and probabilistic techniques proposed for Uncertainty Quantification, including Stochastic Galerking, Stochastic Collocation, Stochastic perturbation, Monte Carlo techniques, sensitivity analysis, worst-case scenario, fuzzy sets, etc.

Uncertainty quantification for chaotic fluid dynamics. **James Glimm** (SUNY at Stony Brook, USA) IC/MT414/010

Chaotic flows are unstable on all length scales and display problematic convergence properties, because new phenomena emerge under mesh refinement. We develop feature extraction methods for shock and mixing dominated flows. We show that the large scale descriptions of the features converge numerically and determine orders of convergence. This is an essential step in uncertainty quantification for chaotic fluid dynamics.

Multiscale stress assessment in random heterogeneous media. **Robert Lipton** (Louisiana State University, USA) IC/MT2516/010

In this talk we discuss new methods for the assessment of the local stress field inside stochastically defined media. Here we show how to make progress on this problem when the length scale of the heterogeneities are smaller than the characteristic wavelength of the boundary data. We show how to apply new optimal lower bounds on local field quantities in order to characterize local stress fluctuations in terms of the statistics of the microgeometry.

Parametric models for processes with continuous samples and applications to linear random vibration. **Mircea Grigoriu** (Cornell University, USA) IC/MT3340/010

Most actions on physical systems are non-Gaussian processes that have continuous samples. Since the output of linear systems to non-Gaussian input is usually non-Gaussian, the classical mean and covariance equations of linear random vibration are insufficient for characterizing system output.

There are no general analytical methods for finding the probability law of the output Y of a linear system subjected to an arbitrary non-Gaussian input X. Current analytical methods provide useful information on the probability law of Y for some special classes of input processes, for example, polynomials of filtered Gaussian, Poisson, and Lévy process. Monte Carlo simulation is the only general method for calculating output statistics for linear dynamic systems in non-Gaussian environment. However, current Monte Carlo algorithms can be inefficient if applied to the analysis of relatively large dynamic systems since they obtain samples of Y from samples of X by numerical integration.

A two-step method is proposed for finding response statistics for linear systems subjected to input processes with continuous samples. First, a sequence of parametric models $X_n(t) = \sum_{i=1}^{n} C_i \varphi_i(t)$, $n = 0, 1, \ldots$, is develop for X, where $\{\varphi_i\}$ is a specified collection of continuous functions and $\{C_i\}$ are random variables. Samples of $\{C_i\}$ can be obtained by minimizing the distance between samples of X and X_n. Second, statistics of the output Y of a linear system to an input X are approximated by those of the output Y_n of the linear system to X_n. Since Y_n is linear in $\{C_i\}$, its statistics can be obtained simply from samples of $\{C_i\}$. Numerical examples are used to illustrate the construction of the proposed parametric models $\{X_n\}$ and the calculation of statistics of $\{Y_n\}$. It is shown that the parametric models $\{X_n\}$ are accurate and the processes $\{Y_n\}$ provide satisfactory and efficient approximations of Y for sufficiently large values of n.

Uncertainty quantification with random-matrix theory. **Daniel Tartakovsky** (UC San Diego, USA), Sondipon Adhikari (University of Bristol, UK) IC/MT3521/010

Consider diffusion (heat conduction) in a highly heterogeneous environment whose diffusion coefficient (thermal conductivity) D is sampled at a few locations throughout a computational domain. The lack of sufficient information about D renders this problem under-defined and, hence, ill-posed. The problem is routinely regularized by treating D as a random field and the corresponding diffusion equation as stochastic. A key feature of this and other similar stochastic problems is that the randomness of system parameters, such as D, is multiplicative. A solution of such stochastic problems requires a closure approximation in all but a few special cases. This is true for either analytical methods (e.g., a closure by perturbation) or direct statistical methods (e.g., the use of a finite number of realizations in Monte Carlo simulations) or numerical methods (e.g., truncation of infinite series in polynomial chaos expansions). The approximate nature of such solutions formally limits their applicability to either mildly heterogeneous or long-correlated environments.

We propose an alternative approach that, in many applications, obviates the need for a closure approximation. It relies on a representation of a stochastic partial differential equation as a system of coupled linear random algebraic equations. To solve such a problem is to find the inverse of the corresponding random matrix. We present an exact analytical method for the inverse of a real symmetric (in general non-Gaussian) random matrix of arbitrary dimension. The proposed method is based on random matrix theory and utilizes the Jacobian of the underlying nonlinear matrix transformation. For steady-state diffusion, exact expressions for the mean and covariance of the system state is obtained exactly in closed form.

IC/MP103/010: Uncertainty quantification in computational science and engineering, II. #2

Organiser: Fabio Nobile (Politecnico di Milano, Italy)
Co-organiser: Raul Tempone (Florida State University, USA)

(For abstract, see session #1 above.)

Dual-based error analysis for uncertainty quantification in a chemical system. **Lionel Mathelin** (LIMSI, France), Olivier Le Maître (Université de Evry, France) IC/MT1774/010

This work is concerned with accurate uncertainty quantification (UQ) in a reduced hydrogen oxidation mechanism involving 7 species and 8 reactions. The uncertainty arises from the inexact knowledge of the reaction rates, which are parameterized using 8 independent random variables. A Stochastic Finite Element (SFE) discretization of the random solution is performed using a stochastic basis of piecewise continuous orthogonal polynomials. Due to the stochastic dimensionality of the problem ($N = 8$), it is essential to properly select the SFE basis in order to minimize the approximation error, while maintaining the basis' dimension as low as possible. To this end, a dual-based *a posteriori* error analysis of the SFE approximation is proposed to construct a refinement/coarsening procedure for the representation, which aims at satisfying a prescribed accuracy criterion. The SFE refinement may consist in increasing the order of some stochastic elements (p-refinement), or by splitting some elements into smaller ones (h-refinement). Straightforward isotropic h-refinement is not an option as it would result in an intractable increase of the SFE basis' dimension. Instead, a directional error estimator is proposed for the selection of the stochastic dimensions requiring refinement. If no refinement direction is found, *i.e.* if the SE's error is balanced between all the stochastic dimensions, a p-refinement is applied. On the contrary, the coarsening procedure is used to merge neighboring SFEs having low a posteriori error estimates, when fine stochastic discretization becomes unneces-

sary during the time-evolution of the chemical system.

Numerical tests show that the proposed methodology allows for a fine control of the solution accuracy and significant savings in the computational resources used (CPU and memory requirement).

Global sensitivity analysis: novel settings and methods. **Michaela Saisana** (Joint Research Centre, Italy), Andrea Saltelli (European Commission, Joint Research Centre, Ispra, Italy) IC/MT2128/010

This presentation wants to be an introduction to global sensitivity analysis (SA). Its ambition is to target an audience unfamiliar with global sensitivity analysis, and to give practical hints about the associated advantages and the effort needed.

We shall review some techniques for sensitivity analysis, including those that are not global, by applying them to a simple example. This will give the audience a chance to contrast each method's result against its own expectation of what the sensitivity pattern for the simple model should be. We shall also try to relate the discourse on the relative importance of model input factors to specific questions, such as *"Which of the uncertain input factor(s) is so non-influential that we can safely fix it/them?"* or *"If we could eliminate the uncertainty in one of the input factors, which factor should we choose to reduce the most the variance of the output?"*

A set of worked examples, e.g. application of global sensitivity analysis to real models, is mentioned briefly to illustrate possible useful practices, and reference is given to the existing literature on the subject. Some most common pitfalls will be mentioned as well.

[1] A. Saltelli, M. Ratto, S. Tarantola and F. Campolongo (2005) *Sensitivity Analysis for Chemical Models*, Chemical Reviews, 105(7) pp 2811 - 2828.

Propagating uncertainty in elliptic problems via a worst scenario analysis. **Fabio Nobile** (Politecnico di Milano, Italy), Raul Tempone (Florida State University, USA), Ivo Babuška (University of Texas at Austin, USA) IC/MT3261/010

Many physical problems are affected by a relatively large uncertainty in the input data and in the coefficients of the underlying mathematical model. In many cases, a full statistical characterization of those uncertainties is impossible to obtain and the only information available is a range where the input data and model coefficients can vary in.

In this work we focus on elliptic PDE's which may feature uncertainty in the coefficients or boundary conditions. Particular attention is devoted to the case of uncertainty in Dirichlet boundary data. We address a deterministic treatment of uncertainty in terms of admissible sets of parameters in the PDE (without introducing any probability measure on these sets) and we aim at identifying the *worst* choice of parameters that leads to the maximum uncertainty in some specific quantities of interest.

The proposed technique for uncertainty quantification and worst-case scenario analysis is based on a perturbation method. It is computationally inexpensive and allows one to account for perturbations in infinite dimensional spaces.

We will present a careful error analysis and numerical examples showing the effectiveness of the methodology.

References

[1] I. Babuška, F. Nobile and R. Tempone, *Worst-case scenario analysis for elliptic problems with uncertainty*, Numer. Math.(2005), 101:185–219

[2] I. Babuška, F. Nobile and R. Tempone, *Propagating uncertainty from boundary conditions in elliptic problems via a worst scenario analysis*, in preparation.

[3] I. Babuška, F. Nobile and R. Tempone, *Worst-case scenario analysis for elliptic PDEs with uncertainty*, EURODYN 2005 Proceedings, C. Soize and G. Schuëller eds.

IC/MP202/010: Multiscale modeling and computation.

Organiser: Olof Runborg (Kungliga Tekniska högskolan, Sweden)
Co-organiser: Yen-Hsi Tsai (University of Texas at Austin, USA)
Co-organiser: Björn Engquist (University of Texas at Austin, USA)

There is an emergence of computational methods for simulating phenomena where the coupling of multiple physical models is essential. The underpinning models typically describe a physical system at different scales, using different variables. In particular, the methods can replace heuristics and empirical observations in coarse scale single physics models by direct numerical simulations of more accurate fine scale models. For example, an atomistic computation may help to evaluate the constitutive equation in a complex fluid. Solving the fine scale equations accurately over relevant macroscopic length and time scales is often too costly. In many cases, sufficient information on the fine scales' influence on the coarse scale dynamics can be obtained by performing spatially localized simulations over short times. This can significantly reduce the numerical complexity so that it is now feasible to treat problems that could not be handled previously in areas such as complex fluids, defect formation in solids, and certain dynamical systems. However, the coupling also introduces new modeling and numerical errors that should be analyzed carefully. These three integrated minisymposia bring applied computational scientists and numerical analysts together for exchange of recent developments and to stimulate further advances in multiscale modeling and computation.

Atomistic and continuum stochastic models for phase change dynamics. **Anders Szepessy** (Royal Institute of Technology (KTH), Sweden) IC/MT3916/010

The dynamics of dendritic growth of a crystal in an undercooled melt is determined by macroscopic diffusion-convection of heat and capillary forces acting on length scales compared to the nanometer width of the solid-liquid interface. Its modeling is useful for instance in processing techniques based on casting. The phase field method is widely used to study evolution of such microstructures of phase transformations on a continuum level; it couples the energy equation to a phenomenological Allen-Cahn/Ginzburg-Landau equation modeling the dynamics of an order parameter determining the solid and liquid phases, including also stochastic fluctuations to obtain the qualitative correct result of dendritic side branching. This lecture presents some ideas, in the spirit of Lax equivalance theorem, to derive stochastic phase field models from atomistic formulations by coarse-graining molecular dynamics and kinetic Monte Carlo methods.

Dynamic density functional theory (DDFT) for nucleation and growth of crystals: atomistic simulations on diffusive time scales. **Axel Voigt** (FZ caesar, Germany) IC/MT3970/010

Classical density functional theory (DFT) is a very successful theory to describe thermdynamics and equilibrium structures of fluids. It is based upon a minimization principle for a free energy density functional and determines the equilibrium ensemble average one body density profile of a classical fluid. Given the success of DFT, it is very appealing to construct a dynamical theory from it. To obtain en equation of motion for the one-body density profile $\rho(\mathbf{x},t)$ an ensemble average over the possible configurations of the system at time t, given an ensemble at $t=0$ is needed. It is assumed that the gradient of the chemical potential $\nabla\mu(\mathbf{x},t)$ is the thermodynamic driving force for the particle current $\mathbf{j}(\mathbf{x},t) = -\Gamma\nabla\mu(\mathbf{x},t)$, where Γ is a mobility function. μ is given by the functional derivative of the Helmholtz free energy functional with respect to the density profile. All together give the continuity equation $\partial_t\rho(\mathbf{x},t) = -\nabla\cdot\mathbf{j}(\mathbf{x},t)$, and provide the basis for DDFT. Equations of this form have been used is various fields and their agreement with results from Brownian dynamics simulations have generally been very good. We are here interested in the dynamics of freezing, in the theoretical understanding of nucleation and the subsequent growth of crystals. In this context the emergence of an ordered phase can be viewed as a transition to a phase in which $\rho(\mathbf{x},t)$ is highly non-homogenous and possesses the spacial symmetries of the crystal. Appropriate truncation of higher order correlation functions in the free energy functional lead to a closed system which forms a higher order nonlinear PDE for $\rho(\mathbf{x},t)$. We thus have constructed a model on an atomistic resolution, which operates on diffusive time scales. Numerical results based on finite elements will be shown to study nucleation and grain growth in BCC and FCC crystals.

A statistical continuum theory of dislocations. **Thomas Hochrainer** (Fraunhofer IWM Freiburg, Germany), Daniel Weygand (Universität Karlsruhe, Germany), Peter Gumbsch (Fraunhofer IWM Freiburg, Germany), Michael Zaiser (University of Edinburgh, UK), Ferenc Csikor (Eötvös Loránd Tudománygyetem, Hungary) IC/MT3873/010

We recently proposed a second order dislocation density tensor which makes the distinction between geometrically necessary and statistically stored dislocations dispensable. It is termed of second order because it contains information on the curvature of the dislocations. We will discuss in detail how this dislocation density tensor is used to derive a statistical continuum theory of dislocations. Furthermore the incorporation of dislocation sources into the framework shall be discussed. Discrete dislocation simulations were used to determine pair correlations in dislocation systems and to derive physically based laws for the evolution and activation of dislocation source.

A multiscale method for epitaxial growth. **Russel Caflisch** (University of California, Los Angeles, USA), Yi Sun (Courant Institute, NYU, USA), Björn Engquist (University of Texas at Austin, USA) IC/MT4989/010

We investigate a heterogeneous multiscale method (HMM) for interface tracking and apply the technique to the simulation of epitaxial growth. HMM relies on an efficient coupling between macroscale and microscale models. When the macroscale model is not fully known explicitly or not accurate enough, HMM provides a procedure for supplementing the missing data from a microscale model. Here we design a multiscale method that couples kinetic Monte-Carlo (KMC) simulations on the microscale with the island dynamics model based on the level set method and a diffusion equation. Numerical results for island growth and step edge evolutions show improved efficiency over pure KMC simulations while keeping the KMC modeling of the internal boundary conditions.

IC/MP729/010: Multiscale modeling and computation: fluids.

Organiser: Yen-Hsi Tsai (University of Texas at Austin, USA)
Co-organiser: Olof Runborg (Kungliga Tekniska högskolan, Sweden)
Co-organiser: Björn Engquist (University of Texas at Austin, USA)

There is an emergence of computational methods for simulating phenomena where the coupling of multiple physical models is essential. The underpinning models typically describe a physical system at different scales, using different variables. In particular, the methods can replace heuristics and empirical observations in coarse scale single physics models by direct numerical simulations of more accurate fine scale models. For example, an atomistic computation may help to evaluate the constitutive equation in a complex fluid.

Solving the fine scale equations accurately over relevant macroscopic length and time scales is often too costly. In many cases, sufficient information on the fine scales' influence on the coarse scale dynamics can be obtained by performing spatially localized simulations over short times. This can significantly reduce the numerical complexity so that it is now feasible to treat problems that could not be handled previously in areas such as complex fluids, defect formation in solids, and certain dynamical systems. However, the coupling introduces new modeling and numerical errors that should be analyzed carefully.

We propose three integrated minisymposia that bring applied computational scientists and numerical analysts together to facilitate the exchange of recent developments and stimulate further advances in multiscale modeling and computation.

Multiscale modeling of fluids. **Weiqing Ren** (New York University, USA) IC/MT2285/010

I will present multicale modeling and computation of complex fluids and microfluidics.

Numerical simulation of nucleation and phase separation coupled with crystallization. **Pingwen Zhang** (Peking University, PR China) IC/MT1806/010

The kinetics of liquid–liquid phase separation and crystallization are simulated based on the double temperature-quench experiments through the time-dependent Ginzburg–Landau equations. Numerical simulations demonstrate that our model can successfully reveal the experimental observations, especially the mechanism of *fluctuation assisted nucleation* in the crystallization process which has been proposed by Han's group in the experimental measurements for the statistical copolymer blends of poly (ethylene-co-hexene) (PEH) and poly (ethylene-co-butene) (PEB). We will also introduce new numerical methods to study the equilibrium states and the nucleation in copolymer melts. We propose a new numerical method which can adjust the periodical region of the equilibrium states automatically. The main idea is to treat the shape of the simulation box as a variable, and then transform the region to a unit box. Although the numerical results are achieved under the Landau–Brazovskii model, it is a general method, and the main advantage of our method is that it can be easily planted in any other theoretic frame like self-consistent field theory. The understand-

ing of the equilibrium state provides the foundation to study the nucleation. Nucleation is the decay of a metastable state via the thermally activated formation and subsequent growth of droplets of the equilibrium phase. We will consider the nucleation in diblock copolymer melts, whose equilibrium phases are well understood. We apply a new numerical method, called the string method, to compute the minimum energy path (MEP). Then from the MEP, we find the size and shape of the critical droplet and the free-energy barrier to nucleation.

Computational studies of nematic liquid crystalline polymers in planar shear flow. **Carlos García-Cervera** (UC Santa Barbara, USA), Hector Ceniceros (University of California, Santa Barbara, USA) IC/MT3241/010

We present fully three-dimensional numerical simulations of the dynamics of the Doi-Marrucci-Greco model for nematic liquid crystals. The model couples the Smoluchowski equation for the orientational distribution function with the Navier-Stokes equations, via a closure approximation. The simulations show the formation and dynamics of roll cells and disclinations, and are in both qualitative and quantitative agreement with recent experiments.

The work presented has been carried out in collaboration with Dr. Harley Klein (Leeds University), Prof. H.D. Ceniceros (UCSB), and Prof. L.G. Leal (UCSB).

Multiscale simulations of dense fluids. **Petros Koumoutsakos** (ETH Zürich, Switzerland) IC/MT1545/010

We discuss the coupling of Molecular Dynamics and continuum models (Navier Stokes and Lattice Boltzmann) for the simulation of liquids. A novel, interface forcing term is introduced to match atomistic and continuum simulations. We demonstrate that this interface forcing term can be extended to particle simulations, such as Dissipative Particle Dynamics, where material properties are distorted in the absence of periodicity. Results of benchmarks problems and flows over nanopatterened surfaces demonstrate the advantages and drawbacks of this approach.

IC/MP729/010: Multiscale modeling and computation: fluids. #2

Organiser: Yen-Hsi Tsai (University of Texas at Austin, USA)
Co-organiser: Olof Runborg (Kungliga Tekniska högskolan, Sweden)
Co-organiser: Björn Engquist (University of Texas at Austin, USA)

(For abstract, see session #1 above.)

Coupling atomistic and continuum models. **Weinan E** (Princeton University, USA) IC/MT3912/010

I will discuss the recent work with Xiantao Li and Weiqing Ren on coupling atomistic and continuum models for modeling solids and fluids. I will discuss issues of stability of numerical algorithms and accuracy across the atomistic-continuum interface. In particular, I will discuss how to treat thermal noise and the effect of statistical noise.

Deterministic spectral solvers for non-conservative non-linear Boltzmann transport equation. **Irene Gamba** (University of Texas at Austin, USA) IC/MT3678/010

We present the implementation of spectral deterministic solvers for non-linear Boltzmann transport problems capable to model energy dissipative flows, such granular gases or elastic gases in presence of thermostat, where non-Gaussian (NESS) states appear as stable homogeneous long time limits. Under these states there are no reliable hydrodynamic systems as asymptotic limits of Boltzmann type equations.

A novel characteristic of this computational approach is the enforcement of conserved quantities by Lagrange multipliers, that makes it work for both energy conservation and energy dissipation as well.

This is work in collaboration with Harsha Tharkabhushanam

Modeling and simulation of micro- and rarefied-gas flow. **Manuel Torrilhon** (ETH Zürich, Switzerland) IC/MT2985/010

Many applications in physics and engineering consider instationary processes of non-equilibrium gas flows in which standard thermodynamics is not valid. Examples range from rarefied gas dynamics to micro-flows in small-scale devices. In these cases the density or scale is so small that the particles of the gas do not collide often enough to produce a thermalized equilibrium. This is often described by the ratio between the mean free path and a macroscopic scale (Knudsen number) which becomes large in non-equilibrium flows.

During this talk we will discuss the mathematical derivation of continuum equations for non-equilibrium gases, based on kinetic gas theory and Boltzmann's equation. A new approach will be presented, which performs an asymptotic expansion around a fixed non-equilibrium. The new equations are highly accurate and fully stable in contrast to common models (Navier-Stokes, Fourier, Chapman-Enskog, Grad, Burnett, etc).

Additionally, some results for applications, like shock wave profiles and shock-density-interactions, will be shown.

Phase transition of a thermally driven Allen–Cahn equation, and solution of the associated optimal control problem. **Mattias Sandberg** (Universitetet i Oslo, Norway) IC/MT4964/010

We will discuss a model problem for phase transitions of a spatially extended system, an Allen-Cahn/Ginzburg-Landau equation perturbed by a small noise term. Via the theory of rare events the probability of transition between the two stable equilibria is, in the limit of vanishing noise, given by the minimizer to an action functional. This minimization may be viewed as an optimal control problem involving the Allen-Cahn equation. A method for approximation of this control problem, including discretization in space and time, is presented. Convergence is proved by employing the Hamilton-Jacobi equations for both the discretized and the original problems, the latter being defined on a space of infinite dimension. The transition proceeds via one or more nucleation events, followed by propagation of domain walls, which will be shown by numerical calculations.

IC/MP728/010: Multiscale modeling and computation: dynamical systems.

Organiser: Yen-Hsi Tsai (University of Texas at Austin, USA)
Co-organiser: Olof Runborg (Kungliga Tekniska högskolan, Sweden)
Co-organiser: Björn Engquist (University of Texas at Austin, USA)

There is an emergence of computational methods for simulating phenomena where the coupling of multiple physical models is essential. The underpinning models typically describe a physical system at different scales, using different variables. In particular, the methods can replace heuristics and empirical observations in coarse scale single physics models by direct numerical simulations of more accurate fine scale models. For example, an atomistic computation may help to evaluate the constitutive equation in a complex fluid.

Solving the fine scale equations accurately over relevant macroscopic length and time scales is often too costly. In many cases, sufficient information on the fine scales' influence on the coarse scale dynamics can be obtained by performing spatially localized simulations over short times. This can significantly reduce the numerical complexity so that it is now feasible to treat problems that could not be handled previously in areas such as complex fluids, defect formation in solids, and certain dynamical systems. However, the coupling introduces new modeling and numerical errors that should be analyzed carefully.

We propose three integrated minisymposia that bring applied computational scientists and numerical analysts together to facilitate the exchange of recent developments and stimulate further advances in multiscale modeling and computation.

Analysis of heterogeneous multi-scale methods. **Björn Engquist** (University of Texas at Austin, USA) IC/MT4195/010

The heterogeneous multi-scale method is a framework for developing computational multi-scale techniques, for example, for coupled atomistic and continuum simulations. The framework is also very useful in the convergence study of a wide class of algorithms for multi-scale problems. We will mainly discuss homogenization problems and stiff dynamical systems.

Numerical integrators for multiscale dynamical systems with stochastic effects. **Eric Vanden-Eijnden** (Courant Institute, NYU, USA) IC/MT1279/010

We will discuss a class of numerical integrators for dynamical systems with multiple time-scales and stochastic effects such as stochastic differential equations or continuous-time Markov jump processes. These integrators build on limiting theorems for singularly perturbed Markov processes and have a cost which is independent of the small parameter measuring timescale separation in the systems – in contrast, the cost of standard integrators would increase as the inverse of this small parameter.

Adaptive stochastic dynamics for the computation of free-energy differences. **Tony Lelièvre** (École Nationale des Ponts et Chaussées, France) IC/MT3742/010

Stochastic dynamics to compute free energy differences are widely used in computational chemistry and biology. Many recent methods rely on complex Markov processes (non-homogeneous or non-linear processes). Examples of such methods are exponential reweighting of non-equilibrium paths (Jarzynski equality) and Adaptive Biasing Force (ABF) techniques. A unifying presentation of adaptive methods is proposed. We also prove the convergence of a certain class of adaptive methods. Finally, we present an efficient implementation of adaptive dynamics using an interacting particle system with birth death processes.

Some numerical studies on the implicit methods for multiscale systems. **Tiejun Li** (Peking University, PR China) IC/MT2683/010

We demonstrate, by a combination of analytical arguments and numerical examples, that implicit stiff ODE (ordinary differential equation) solvers are not effective for dynamical systems with multiple time scales when the quasi-equilibrium distributions for the fast variables are not Dirac distributions. This is due to the fact that such implicit methods cannot correctly capture non-Dirac invariant distributions when the time step size is much larger than the relaxation time of the system.

IC/MP728/010: Multiscale modeling and computation: dynamical systems. #2

Organiser: Yen-Hsi Tsai (University of Texas at Austin, USA)
Co-organiser: Olof Runborg (Kungliga Tekniska högskolan, Sweden)
Co-organiser: Björn Engquist (University of Texas at Austin, USA)

(For abstract, see session #1 above.)

Chebyshev methods for stiff stochastic problems. **Assyr Abdulle** (University of Edinburgh, UK) IC/MT2751/010

Stiff stochastic systems play a major role in a wide range of applications. For problems with scale separation, explicit multiscale methods have recently been proposed. Implicit methods are usually advocated for stiff problems when fast and slow dynamics cannot be separated. In this talk we discuss a new class of explicit methods for the efficient treatment of stiff stochastic problems without scale separation.

This is a joint work with S. Cirilli (Geneva).

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Multiscale methods for the wave equation. **Olof Runborg** (Kungliga Tekniska högskolan, Sweden), Björn Engquist (University of Texas at Austin, USA) IC/MT3420/010

We consider the wave equation in a medium with a rapidly varying speed of propagation. We construct a multiscale scheme based on the heterogeneous multiscale method, which can compute the correct coarse behavior of wave pulses traveling in the medium, at a computational cost essentially independent of the size of the small scale variations. This is verified by theoretical results and numerical examples. The work is in collaboration with Bjorn Engquist and Henrik Holst.

A multiscale method for a class of stiff ODEs with polynomial right-hand-side. **Yen-Hsi Tsai** (University of Texas at Austin, USA) IC/MT3374/010

We consider a class of ODE systems with highly oscillatory components. Through resonances among these oscillations, nontrivial slow behavior of a given system is generated. To achieve efficient solution without resolving the oscillations everywhere, the resonances in the system must be consistently modeled. We present our strategy for detection of the resonance and determination of a set of slow variables using the dynamics of the given oscillatory system. The slow variables are then integrated using an algorithm developed under the Heterogeneous Multiscale Method framework.

This is joint work with Bjorn Engquist and Gil Ariel

Application of the heterogeneous multiscale methods to highly-oscillatory ODEs. **Richard Sharp** (University of Texas at Austin, USA) IC/MT2838/010

The Heterogeneous Multiscale Methods (HMM) is a framework for efficiently and accurately treating multiscale problems. Frequently, the macroscopic quantities of interest in a problem depend on the microscopic evolution of a system. Depending on the problem, it may be necessary to fully resolve the microscale, because it is not possible to accurately coarsen this description and write a macroscopic model. In materials science for example, crystal growth depends on the the ease with which a single molecule can be added to the lattice, but semiconductor devices produced this way are bulk materials. A fully resolved atomistic simulation is too computationally expensive to achieve, and even if it were, the result would need further processing to extract the electrical properties of interest. A strength of HMM style algorithms is that they do not require a specific macroscopic model in order to track macroscopic variables. Instead, such algorithms exploit scale separation to extract macroscopic information from a limited number of local microscopic simulations. Significant challenges lie in identifying an appropriate set of macroscopic variables, and in the exchange of information between the different scales of the problem. I will present recent applications of the HMM to highly oscillatory ODEs, including a driven pendulum and more general autonomous stiff systems. In this setting, the highly oscillatory solution to the microscopic problem converges weakly to a relatively smooth average solution, as scale separation is increased. The slow solution can be simulated with a relatively long time step when a self-consistency condition is used to reinitialize the microscopic model after each update of the macroscopic data.

IC/MP256/015: Numerical simulation of plasmas.

Organiser: James Rossmanith (University of Wisconsin, Madison, USA)
Co-organiser: Andrew Christlieb (Michigan State Univsersity, USA)

Plasmas are ionized gases that appear in a wide range of applications including astrophysics and space physics, as well as in laboratory settings such as in magnetically confined fusion. Modeling and understanding the basic phenomenon in plasmas has long been a topic in scientific computing, yet many problems remain far too numerically intensive for modern parallel computers. The main difficulty is that plasmas span a wide range of spatial and temporal scales, requiring modeling tools from both fluid and kinetic theory. This minisymposium aims to give an overview of the state of the art in plasma simulations; and as such, it touches on variety of topics ranging from advanced simulation methods for ideal MHD to fully kinetic simulation techniques. Furthermore, a variety of application areas will be addressed including astrophysics, spacecraft design, and magnetically confined fusion.

Computing the radiation source term in the system of radiation-magnetohydrodynamics in 3D. **Andreas Dedner** (Universität Freiburg, Germany) IC/MT2885/015

In this talk we present a scheme for solving the equations of radiation magnetohydrodynamics (RMHD) in three space dimensions, a non–linear system of balance laws combining the effects of magnetohydrodynamics (MHD) and mon-local energy transport through radiation. The starting point of our presentation is a standard explicit second order finite-volume scheme for the MHD equations on both structured and unstructured locally adapted parallel grids. To add the energy transport through radiation we have to compute the radiation source term in the balance law for the total energy density:

$$Q_{\text{rad}} := \rho\kappa(\rho, T) \int_{S^2} (S(T) - I_\mu)\, d\mu$$

We denote with ρ and T the density and the temperature of the plasma, respectively, and I_μ denotes the radiation intensity in direction $\mu \in S^2$. Since in our application hydrodynamic time scales are much smaller than the time scale in the radiation transport, the radiation intensity is modeled using the stationary radiation trasport (RT) equation:

$$\mu \cdot \nabla I_\mu + \rho\kappa(\rho, T) I_\mu = \rho\kappa(\rho, T) S(T)$$

Solving this equation even for a small number of directions μ leads to a considerable increase in computational cost - at least 70% of the computational cost for the full coupled system is spent in computing the radiation source term. Thus a highly efficient scheme for approximating the radiation source term Q_{rad} is an essential part of any method for solving the fully coupled RMHD equations. This will be the main focus of our presentation. We present results concerning the convergence of the numerical scheme and numerical tests, comparing our *extended short characteristics* scheme with some standard schemes found in the literature, e.g., the discontinuous Galerkin approach. Since the approximation of the radiation intensities in a fixed direction μ is not so crucial as the approximation of the radiation source term Q_{rad} in the energy balance law, we will concentrate on this aspect of the numerical schemes. We conclude our presentation with a study of the parallelization strategy for distributed memory computers that we use in our 3d code.

On electric light arc simulations with MHD. **Manuel Torrilhon** (ETH Zürich, Switzerland) IC/MT3022/015

Light arcs appear as electrical discharges between two conductors with strong difference in potential. The archetype of a light arc is the lightning in a thunderstorm. But light arcs are also found in various engineering applications like circuit breakers. In a light arc the gas is ionized and turned into a plasma with high electrical conductivity that interacts with electric and magnetic fields. Hence, simulations of light arcs are examples for an industrial need of magnetohydrodynamics. This talk will present basic physical characteristics of light arcs with various simplified model problems. The fundamental driving force is the interaction between temperature and electric current. We also discuss the light arc as a multi- physics phenomena. Difficulties are strongly varying electrical conductivity, influence of external fields and radiation transport, as well as turbulence. Parts of the talk will present results from an ongoing project on full scale light arc simulations in the Seminar for Applied Mathematics at ETH Zurich.

IC/MP256/015: Numerical simulation of plasmas. #2

Organiser: James Rossmanith (University of Wisconsin, Madison, USA)
Co-organiser: Andrew Christlieb (Michigan State Univsersity, USA)

(For abstract, see session #1 above.)

Volumetric point insertion for grid-free Lagrangian particle methods. **Andrew Christlieb** (Michigan State Univsersity, USA) IC/MT2372/015

Plasmas (ionized gases) have rich and complex behavior which often need multiple lines of attack to fully understand their rich dynamics. Depending on the length scales involved, the plasma may be described by either a kinetic or a fluid model, the kinetic model being the more fundamental of the two. In this talk we will give a brief overview of the relation between these two models and then discuss grid-free Lagrangian particle methods for kinetic plasma problems using adaptive volumetric point insertion. Specifically, our talk will discuss the application of this approach to the Vlasov–Poisson system, a kinetic model, and the warm two stream instability. In addition, a comparison with grid-based Lagrangian particle models will be presented. At the end of the talk we will briefly discuss our plans for developing a multi-scale plasma model spanning the entire range of length scales from kinetic to fluid models.

Residual distribution schemes for astrophysical plasmas. **James Rossmanith** (University of Wisconsin, Madison, USA) IC/MT2020/015

An important problem in modern astrophysics is to understand the accretion of ionized gases onto a black hole and the formation of relativistic jets that can sometimes result from this process. Even with significant simplifying assumptions, including that the spacetime is static and that the accreting dust obeys the relativistic MHD equations, accurate numerical computations of such flows are still quite challenging to obtain. Some of the difficulties include the strong curvature of spacetime near the event horizon, the divergence-free condition on the magnetic field, the complex equation structure due to the Lorentz factor, and non-trivial balances between flux gradients and geometric source terms. In this talk we will describe an effort to develop genuinely multidimensional, high-resolution, shock-capturing schemes on unstructured grids for solving the relativistic MHD equations. The resulting method will be applied to several axisymmetric computations of black hole accretion.

Hybrid Monte-Carlo methods for fluid and plasma dynamics. **Russel Caflisch** (University of California, Los Angeles, USA) IC/MT2070/015

For small Knudsen number, simulation of rarefied gas dynamics by the DSMC method becomes computationally intractable because of the large collision rate. To overcome this problem we have developed a hybrid simulation method, combining DSMC and a fluid dynamic description into a single seamless method. The molecular distribution function f is represented as a linear combination of a Maxwellian distribution M and a particle distribution g; i.e., $f = bM + (1-b)g$. The density, velocity and temperature of M are governed by fluid-like equations, while the particle distribution g is simulated by DSMC. In addition there are interaction terms between M and g. The coefficient b is determined automatically, by a thermalization approximation. Numerical results will be presented to demonstrate the validity of this method, as well as the acceleration that it provides over DSMC. This method has been extended to simulation of Coulomb collisions in a plasma. For this extension, the underlying Monte Carlo method is Nanbu's method for Coulomb collisions.

High-resolution central schemes for kinetic and fluid plasma models. **Jorge Balbás** (University of Michigan, Ann Arbor, USA) IC/MT3003/015

In this work we present high-reslution central schemes for two-species plasmas described by the microscopic Vlasov kinetic model and by the macroscopic Euler-Poisson fluid model. While the microscopic model provides a rather accurate description for collisionless plasmas, numerical simulations require the discretization of each component of the velocity field as one more variable in phase space which, in turn, demands considerable computer time and power. Alternatively, one can consider the Euler-Poisson equations, which consist of a hyperbolic system of conservation laws for each species with an inhomogeneous term that coples the two systems through the electric field (Poisson Equaton); a model resulting from taking the first three moments of Valsov equation. Although the description provided by the fluid model is not as accurate as its microscopic counterpart, it is still adequate for many plasma simulations and considerable less computationally expensive to simulate.

Finite volume numerical schemes for both models have been recently developed and employed so as to asess the validity of the fluid model by comparing the results obtained wtih this to those obtained with its kinetic counterpart. To this end, we propose the development of finite volume schemes based on central differencing. Central schemes avoid the costly use of (approximate) Riemann solvers for the fluid model, resulting in simple –yet robust– *black box* type numerical schemes.

IC/MP323/015: Modeling the mechanics of the cardiovascular system.

Organiser: Joakim Sundnes (Simula Research Laboratory, Norway)
Co-organiser: Gerhard Holzapfel (Royal Institute of Technology (KTH), Sweden)

For several decades nonlinear solid mechanics has been applied to the cardiovascular system. A continuous development in mathematical techniques and computer hardware has occurred in parallel with a gradually improved knowledge of biological behavior and material properties of soft tissues. This has allowed scientists to build more and more complex and realistic models of this vital system, and has resulted in increasingly accurate model predictions and improved (patho)physiological understanding, as well as direct applications in clinical practice. Important examples include design of medical devices such as artificial heart valves and heart assist devices, and the development of vital procedures such as heart transplants and bypass surgery. However, in spite of these success stories, there are still many unresolved issues related to both biology-specific formulations and to challenges of modeling the material behavior of soft biological tissues. From a viewpoint of computational mechanics, particular challenges include finite strains, nonlinear elastic or viscoelastic material behavior, anisotropy, fluid-structure interaction and the formulation of contact problems including large sliding. In this minisymposium we address solid mechanics modeling of the cardiovascular system, with particular focus on mathematical and computational aspects. We will touch upon several active research areas, spanning from the development of constitutive relations for passive material behavior, through mathematical modeling of active forces developed in

muscle tissues, to addressing the computational challenges involved in solving systems of strongly nonlinear partial differential equations. We will also describe some of the possible applications of the models for clinical work and biomedical science.

Computational techniques for heart muscle mechanics. **Joakim Sundnes** (Simula Research Laboratory, Norway) IC/MT2292/015

The heart occupies the most central role of the cardiovascular system, with the crucial role of supplying a continuous flow of blood through the vast network of vessels composing the circulatory system. Mathematical models of the heart in health and disease is an increasingly important tool for improving our understanding of this vital organ, and thereby help to reduce health problems and costs related to cardiovascular disorders.

In this talk we give an overview of computational challenges and techniques related to modelling the mechanical function of the heart muscle. Models applied for this purpose vary in complexity from the simplest pressure-volume relations based on a given time varying elastance, to systems of differential equations that give a detailed description of cardiac electromechanical interaction.

The primary focus of the talk will be on finite element modeling of the heart muscle, which includes modeling the passive mechanical properties of the tissue as well as the active muscle contraction and its coupling to electrophysiology. The heart muscle is normally modeled as a hyper-elastic material, with strongly non-linear and anisotropic material behavior. The resulting mathematical model consists of a large-strain elasticity equation, which is coupled to DAE systems that describe electro-chemical reactions on cell level, and also to a system of PDEs that describe the conduction of the electrical signal in the tissue. We discuss some approaches for solving this system, which offer a varying degree of coupling and feedback between electrophysiology and mechanics. We also discuss different approaches for coupling the heart muscle models to the rest of the circulatory system. The latter topic will also be covered in more detail in the other talks of the minisymposium.

Ventricular interaction quantified with a novel multi-scale cardiovascular model. **Roy Kerckhoffs** (UC San Diego, USA), Maxwell Neal (University of Washington, USA), James Bassingthwaighte (University of Washington, USA), Jeffrey Omens (UC San Diego, USA), Andrew McCulloch (UC San Diego, USA) IC/MT3354/015

Ventricular interaction (VI) in the heart is the influence of function of one ventricle on the other. Direct VI (DVI) is modulated through the septum and pericardium, while indirect VI (IVI) is referred to as interaction through the circulation. It is difficult however, to separate VI in components DVI and IVI. To investigate VI, a novel multi-scale model of the canine cardiovascular system was developed, that couples an anatomically detailed 3-D finite element model of the ventricles with a closed loop lumped model of the pulmonary and systemic circulations. Multiple beats of a normal heart were simulated, followed by pulmonary artery constriction (PAC).

Methods

The myocardium had nonlinear passive and dynamic active material properties. Both atria were included in the lumped model as time-varying elastances. Hence, the model encompassed levels of the myocyte, tissue, organ, and system. VI was quantified by computing ventricular co-compliances, i.e. the volumic changes in each ventricle due to a pressure change in the other ventricle (CRL=dVR/dPL and CLR=dVL/dPR). This was done at every time step with finite differences by perturbing ventricular pressures.

Results

CLR and CRL varied throughout the cardiac cycles. After PAC, diastolic values changed acutely from -5.7 to -6.5 ml/mmHg, due to an abrupt change in DVI. Over time, CLR and CRL became more negative (-7.4 ml/mmHg), due to IVI.

Conclusions

- VI was quantified using co-compliances. - Using a novel multi-scale cardiovascular model, VI was investigated. VI increased after PAC. - The model is likely to be useful in investigating VI, among others, in many clinical settings.

Stent modelling: application to percutaneous pulomnary-valve implantation. **Francesco Migliavacca** (Politecnico di Milano, Italy), Silvia Schievano (University College London, UK), Claudio Capelli (Politecnico di Milano, Italy), Lorenza Petrini (Politecnico di Milano, Italy), Gabriele Dubini (Politecnico di Milano, Italy), Philipp Bonhöffer (University College London, UK) IC/MT1463/015

Percutaneous pulmonary valve implantation (PPVI) is a catheter-based technique for treating pulmonary valvular disease. Stent fracture is a recognized complication following PPVI. In our series (n=123) we have seen stent fractures occur in 26 patients: 4/10 patients treated with an early generation device and 22/113 with a new design stent. Many different factors play a role in the generation of device fracture including: stent material and design, the nature of the implantation site and stress induced by the functioning valve. The aim of this work is to study some of the factors responsible for stent fracture, by means of finite element analyses (FEA).

METHODS: All patients underwent X-ray investigation following PPVI, at different intervals of time. When fractures were detected, the exact sites of fractures were analyzed from the X-ray films. CAD model of two different stents were designed on the basis of data supplied from the company. The former is a balloon expandable stent, from platinum-10

RESULTS: At X-rays investigation, the early generation stents led to fractures at the strut intersections. The FEA show that the platinum stent presents highest stresses at the same points, proving that this location is more subjected to fracture. In the new design stent, fractures occurred more frequently next to the ends of gold welds. The model shows as the gold reinforces the crossing sections of the platinum device protecting them from fracture. However, the straight platinum parts of this stent present higher stresses then the device without gold welds, because of the reinforcement itself. Indeed, the gold welds create geometrical and material discontinuities. Therefore, the fracture occurs just distal to the welds.

CONCLUSIONS: The finite element method is an important technique to understand stent behaviour and integrity and may aid device design and material before many prototypes are actually manufactured.

Thin-valve simulations with Lagrange multipliers. **Jean-Frédéric Gerbeau** (INRIA Rocquencourt, France), Nuno Diniz dos Santos (INRIA Rocquencourt, France) IC/MT814/015

We present an approach based on Lagrange multipliers to approximate thin valve movements in an incompressible fluid. This strategy allows very large displacements, can be mixed with an Arbitrary Lagrangian Eulerian formulation and is able to tackle changes in the topology of the problem, such as contact. We propose an efficient partitioned algorithm which keeps the fluid and the structure solvers independent. Moreover the algorithm is able to manage contacts without asuming that the structure solver includes contact capabilities. Numerical validations and comparisons with other methods will be presented.

IC/MP701/015: Numerical and asymptotic methods in kinetic-gas theory.

Organiser: Manuel Torrilhon (ETH Zürich, Switzerland)

Kinetic gas theory is the classical non-equilibrium theory of gases based on Boltzmann's equation. It relies on a stochastic description of the particles of the gas and their coarse-grained interaction. Nowadays, applications of kinetic gas theory can be found over a wide range of fields in science and engineering, like plasmas, granular media, semi-conductors, traffic flow and biological modelling. The various kinetic equations still represent a serious challenge with respect to both mathematical theory and numerical methods.

This minisymposium focuses on asymptotic and computational approaches, especially for Boltzmann's equation. Here, the asymptotic theory considers the derivation of continuum models from the kinetic equation valid for small and moderate non-equilibrium. Scaling parameter is the Knudsen number, ie the ratio of mean free path and macroscopic length. Various models and asymptotic theories have been proposed but stability and accuracy remains difficult to obtain. Computational methods have to handle the high dimensionality due to the phase space description as well as non-trivial collision interactions. Hybrid schemes may be able to combine the efficiency of asymptotic models with the accuracy of direct solvers.

Beyond Navier–Stokes: constructing hydrodynamic models to capture unusual rarefied-gas flow phenomena. **Jason Reese** (University of Strathclyde, UK) IC/MT2988/015

I will describe recent and ongoing work at the University of Strathclyde, Glasgow, Scotland, UK, into the new fluid dynamics needed for very high-speed or micro- and nano-scale gas flows. While these are application areas of emerging technological importance, remarkably there is currently no sufficiently accurate and computationally efficient fluid dynamic model. This is because the conventional Navier-Stokes fluid equations do not allow for the local thermodynamic non-equilibrium that makes the behaviour of these rarefied gas flows uniquely complex.

In this talk I will focus on our work on capturing two fundamental aspects of these flows: gas velocity slip at solid surfaces, and the associated Knudsen layer extending from the solid surface into the flow. I will describe the successes and failures of various hydrodynamic models (derived from kinetic theory) being developed to capture this non-equilibrium flow physics, and give examples of current test applications in both hypersonics and micro gas flow situations.

Stabilizing the Burnett fluid dynamics equations. **Lars Söderholm** (Kungliga Tekniska högskolan, Sweden) IC/MT2992/015

The Burnett equations, the equations to second order in the Knudsen number derived by the Chapman–Enskog method, suffer from the unphysical Bobylev instability. A crucial step in the Chapman-Enskog procedure is the use of the approximate conservation laws to replace some time derivatives by space derivatives, we call them formal time derivatives.

It is, however, consistent with the approximation to partly revert this replacement in the resulting expressions for the viscous pressure and heat current. The formal time derivative (denoted by a subscript 0) of the traceless rate of deformation tensor is replaced by a linear combination of the real time derivative and the formal time derivative (α is a parameter)

$$\frac{D_0\mathbf{S}}{Dt} \to (1-\alpha)\frac{D\mathbf{S}}{Dt} + \alpha\frac{D_0\mathbf{S}}{Dt}$$

It is shown that equations that are stable temporally as well as spatially can be achieved choosing α appropriately. The resulting momentum equation is (dots denote nonlinear Burnett terms)

$$\rho\{\mathbf{1}-(\omega_3-\omega_2)\frac{\mu^2}{p\rho}[\frac{1}{2}(\triangle\mathbf{1}-\nabla\nabla)+\frac{2}{3}\nabla\nabla\}\cdot\frac{D\mathbf{v}}{Dt} = -\nabla p+2\nabla\cdot(\mu\mathbf{S})+\omega_3\frac{\mu^2}{\rho^2}\frac{2}{3}\triangle\nabla\rho+..$$

The use of multiple time scales approximation will also be briefly discussed.

The Boltzmann equation and its fluid-dynamic limits: numerical studies. **Hans Babovsky** (TU Ilmenau, Germany) IC/MT3343/015

Recently, a class of discrete kinetic models have been proposed [1,3] emerging from the Boltzmann equation through the choice of a special hexagonal discretization. These have turned out a useful tool for the (at least qualitative) numerical simulation of rarefied gas dynamics in the transition regime to fluid dynamics [2,3].

The Boltzmann equation allows for a variety of scaling limits ranging from the Euler to the Navier–Stokes equations and covering compressible as well as incompressible flows. A review of recent results is contained in [4]. In the talk we will demonstrate the above model as being capable of approaching the diverse hydrodynamic limits. Thus the whole spectrum of scaling limits is covered by one single algorithm which provides a good basis for comparing flow patterns obtained for different parameter regimes. The talk discusses a couple of test cases.

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The lattice-Boltzmann hierarchy: turbulence, microflows and renormalization. **Ilya Karlin** (ETH Zürich, Switzerland) IC/MT3809/015

I will review recent developments [1-5] in the lattice Boltzmann models, with a special emphasis on near-continuum and gas micro-flow simulations. Topics covered include: derivation of the lattice Boltzmann hierarchy of kinetic models, high Reynolds number simulations, exact solutions, thermal models and multi-component mixtures including surface reactions, boundary conditions and implementation issues.

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IC/MP38/015: Computational issues in relativistic quantum chemistry.

Organiser: Gabriel Turinici (Université Paris Dauphine, France)
Co-organiser: Mathieu Lewin (Université Cergy-Pontoise, France)

The main goal of this minisymposium is to present various aspects of computational Relativistic Quantum Chemistry. Relativistic Quantum Chemistry aims at modelling and simulating matter at the microscopic scale, taking into account fine effects encountered by the core electrons in heavy atoms (like Gold or Uranium). These effects have to be considered for an accurate description of the chemical behaviour of the corresponding atoms or molecules. Different types of numerical methods have been developed and are used today by chemists or physicists. But one must admit that the understanding of the relativistic models is not as deep as for the models neglecting these effects. Mathematically speaking, the main difficulties are created by the spectrum of the Dirac operator, which is not bounded by below. Mathematical analysis of the undersying models can help to propose more robust and efficient computational procedures to address these problems. The idea of the minisymposium is to put together specialists from different fields, two from mathematics (nonlinear analysis and numerics) and two from quantum chemistry.

Computation of approximate energy states in relativistic quantum chemistry. **Maria Esteban** (Université Paris-Dauphine, France) IC/MT2853/015

In this talk will be presented numerical computations of energy states for Dirac operators appearing in the modelling of atoms and molecules when relativistic effects are taking into account. These computations are done by using an algorithm based on exact variational characterization of the eigenvalues of Dirac operators, with or without the presence of external magnetic fields.

Spontaneous particle creation within the external field approximation of QED. **Nikodem Szpak** (Max-Planck-Institut Potsdam, Germany) IC/MT3160/015

It is expected that strong electromagnetic fields in QED may lead to destabilization of the vacuum, its decay and spontaneous production of an electron-positron pair if the strength of the electric field exceeds some threshold. We study the problem within an external field approximation of QED in presence of time-dependent external fields and define the spontaneous particle creation via the adiabatic limit. We consider some model fields, which we solve analytically or numerically, in order to explain the subtlety of the effect and to recognize problems appearing in its proof. We conclude by characterizing when the effect can exist in a stable way and when it becomes unstable w.r.t. small perturbations."

The quasi-energy formalism of density-functional theory. **Trond Saue** (Ecole Nationale des Ponts et Chaussées, France) IC/MT3169/015

Density-functional theory (DFT) treats electron correlation efficiently at low computational cost and has therefore become the dominant method in the field of theoretical chemistry. The rigorous foundation of DFT was provided by the Hohenberg-Kohn (HK) theorem and its practical realisation by the Kohn-Sham scheme . The HK theorem establishes a one-to-one correspondence between the (non-degenerate) ground state density and an external scalar potential, usually the electrostatic potential of fixed nuclei, and requires a minimisation principle for its proof. The extension to time-dependent phenomena, including the calculation of response properties as well as excitation energies, was established through the Runge-Gross theorem. This theorem establishes a one-to-one correspondence between a time-dependent external scalar potential and the density of any state provided that the exact initial wave function is given. The Runge-Gross theorem uses a Taylor expansion in time of the scalar potential and does not hold for an adiabatically switched-on static potential. As pointed out by van Leeuwen, the definition of a time-dependent exchange-correlation (xc) potential of some action, in analogy with the definition of the static exchange-correlation potential as the functional derivative of the xc energy with respect to the density, may lead to problems with causality. An alternative approach imposes periodic boundary conditions on the external potential and tries to generalize the HK theorem through Floquet theory. It introduces the quasienergy by extension of the Hilbert space by time averaging. A minimisation principle for the quasienergy has been suggested, but not rigorously proven, by Sambe. In my talk I will discuss the challenges in basing time-dependent DFT (TD-DFT) on Floquet theory.

Reduced-basis methods in RQC. **Yvon Maday** (Université Pierre et Marie Curie, France) IC/MT3011/015

Reduced basis methods allow to approximate accurately and rapidly the solution to general partial differential equation by making use of ad'hoc discrete spaces, built in an off line stage and used online to new situations.
These methods have been introduced in different context: structural mechanics, fluid flows, thermal problems and more recently in quantum chemistry context.

We shall present in this talk new results in relativistic context and illustrate the features of this new method.

IC/MP109/015: Undergraduate computational science and engineering education.

Organiser: Peter Turner (Clarkson University, USA)
Co-organiser: Ignatios Vakalis (California Polytechnic and State University, USA)

Computational Science and Engineering (CSE) is a rapidly growing multi-disciplinary area with connections to the sciences, engineering, mathematics and computer science. CSE is a legitimate and important academic enterprise, even if it has yet to be formally recognized by a number of institutions.
The undergraduate arena is the most important segment of the educational pipeline, since it prepares teachers for the HS environment, invigorates students to pursue graduate studies in cutting edge technical fields, and produce a vast number of future employees for industry and the "knowledge based" economy. Thus it is critical that CSE curricula/ programs are a viable option for every undergraduate student.

The minisymposium will concentrate on: i)model programs of undergraduate computational science and computational engineering programs (USA and Europe); ii)sample undergraduate research experiences and connections to curricula; and iii)needs of industry for CSE undergraduate majors. Key ideas from the upcoming SIAM report will be presented. Sufficient time will be alloed for audience interactions and comments.

Internships and work experience in undergraduate CSE education. **Angela Shiflet** (Wofford College, USA), Peter Turner (Clarkson University, USA) IC/MT5014/015

An internship or work experience can be the climax of a CSE undergraduate's education. With exposure to many new ideas, techniques, and applications at another institution, such an experience can greatly broaden and deepen the student's understanding of computational science and make the classroom education more meaningful. Moreover, work with a professional computational science team and contacts made during the summer can greatly enhance opportunities and options available to the CSE undergraduate.

Keeping CSE curricula focussed. **Ulrich Rüde** (Universität Erlangen–Nürnberg, Germany) IC/MT3723/015

The courses of Computational Science and Engineering programs are typically given by a faculty spread across different departments and institutes and therefore by specialists in their own disciplines. These instructors often follow their own scientific interests and not necessarily those of an genuine education in CSE. Thus there is a danger that depending on the political constellation at a university, a CSE program may degenerate away from CSE into a a conventional degree program. This is typically based on misconceptions among the faculty of what CSE should be about. This talk will attempt to define a set of core skills that CSE programs should teach.

Undergraduate CSE: the SIAM report and research experiences for undergraduates. **Peter Turner** (Clarkson University, USA) IC/MT3456/015

This talk will begin with an introduction to the recently completed SIAM Working Group Report on Undergraduate Computational Science and Engineering. This report covers several aspects including program and course content, different types of undergraduate CSE programs and the desire for research experience within them. The report documents the rapid increase in interest in such undergraduate CSE programs, which can vary from complete baccalaureate majors, through minors or tracks, to just a few courses which can be included in other majors. One of the principal findings and recommendations was the encouragement of internships or other forms of professional or research experience as an important component. Such experiences are valuable in their own right in undergraduate education in general but have a particular role in helping our students understand at first hand the interplay among the various component disciplines that contribute to successful computational science or engineering projects.

IndustrySs need for computational scientists and engineers. **Kirk Jordan** (International Business Machines (IBM), USA) IC/MT3657/015

Computation plays ever increasing and vital role in industry in many scientific areas; from modeling of gas turbines for jet engines to decrease testing to biological models for heart disease to speed clinical trials. In industry, there is an increasing reliance on computational models and simulations. The need to for industry technical and managerial staff who understands computational science and engineering is increasing for companies to remain competitive in today's world. To emphasize this, I will briefly describe a few examples of industry's trend toward simulation and modeling. As this trend continues, industry will increasingly seek individuals with a computational science and engineering background. I will briefly describe what industry might be looking for when seeking to hire an individual with a computational science and engineering background. In closing, I will try to briefly describe how industry works and how to have an impact there.

IC/MP120/025: Level-set methods: current development and applications.

Organiser: Yen-Hsi Tsai (University of Texas at Austin, USA)
Co-organiser: Frédéric Gibou (UC Santa Barbara, USA)
Co-organiser: Stanley Osher (University of California, Los Angeles, USA)

Several problems that arise in science and engineering can be formulated as a front evolution between two (or more) phases. Examples include solidification problems, dendritic growth in materials science, free surface flows, and multiphase flows, to cite a few. One of the main the difficulties in solving such problems comes from the fact that the interface location must be computed as part of the solution to the underlying equations.

Since their inception, level set methods have been extremely successful in tackling these problems. In this minisymposium, the focus will be given to recent advances in the core level set algorithms as well as their applications. Specifically, the core algorithm will cover topics on adaptivity, volume conservation, and solving inverse problems. Applications will include multiphase flows, high frequency wave propagation and shape optimization.

This minisymposium will offer an excellent opportunity for researchers to learn about a wide variety of recent developments in the computational aspects of level set methods as well as their applications and will stimulate cross-pollination between disciplines.

Applications of implicit functions to finite volume discretizations of PDE. **Peter Schwartz** (Lawrence Berkeley National Laboratory, USA), Philip Colella (Lawrence Berkeley National Laboratory, USA) IC/MT3411/015

We address the problem of constructing implicit representations of propagating fronts in fluids. Our interest lies in coupling such representations to second order accurate volume of fluid discretizations of PDE with time-dependent boundaries. Here, we focus on two issues:

1. A discretization of the Hamilton–Jacobi PDE appropriate to interface tracking in fluids problems, which leads us to also consider second-order accurate methods for narrow band formulations of the eikonal equation.
2. An algorithm that uses implicit functions for calculating geometric data, second order in space and time, that can be coupled to second-order accurate discretizations of fluid equations on both sides of the zero level set.

A second-order accurate level-set method on non-graded adaptive Cartesian grids. **Chohong Min** (KyungHee University, Republic of Korea) IC/MT3645/025

We present a level set method on non-graded adaptive Cartesian grids; i.e., grids for which the ratio between adjacent cells is not constrained. We use quadtree and octree data structures to represent the grid and a simple algorithm to generate a mesh with the finest resolution at the interface. In particular, we present:

(1) a locally third-order accurate reinitialization scheme that transforms an arbitrary level-set function into a signed distance function;
(2) a second-order accurate semi-Lagrangian methods to evolve the linear level-set advection equation under an externally generated velocity field;
(3) a second-order accurate upwind method to evolve the non-

linear level-set equation under a normal velocity as well as to extrapolate scalar quantities across an interface in the normal direction; and
(4) a semi-implicit scheme to evolve the interface under mean curvature.

Combined, we obtain a level set method on adaptive Cartesian grids with a negligible amount of mass loss. We propose numerical examples in two and three spatial dimensions to demonstrate the accuracy of the method.

ENO schemes for adaptive grids. **Thomas Cecil** (University of Texas at Austin, USA) IC/MT3433/025

We introduce high order ENO schemes which can be applied on adaptive grids. These schemes are simple modifications of those used on uniform grids and can be applied to hyperbolic problems and Hamilton-Jacobi equations arising in level set flows.

Flexible Matlab implementation of the toolbox of level-set methods. **Ian Mitchell** (University of British Columbia, Canada) IC/MT4300/015

The Toolbox of Level Set Methods is a collection of Matlab routines providing high order accurate finite difference approximations on Cartesian grids in any number of dimensions, although computational cost and visualization make dimensions four and higher a challenge. The modular design of the toolbox makes it easy to try out new level set algorithms, as will be shown by the simple addition of a collection of explicit RK integrators and monotone approximations for degenerate second order spatial terms. We will also demonstrate how the toolbox permits quick and easy experiments with state of the art level set algorithms, and some of the extensive set of examples that are included with the software release. The toolbox and all of its source code is available from the author's web site.

IC/MP67/010: Computational science and engineering (CSE).

Organiser: Kaspar Nipp (ETH Zürich, Switzerland)
Co-organiser: Hans-Joachim Bungartz (TU München, Germany)
Co-organiser: Oskar von Stryk (TU Darmstadt, Germany)

Today, many problems in science and engineering can only be treated using computer-based modelling and simulation. Simulation permits studying complex systems which would be too expensive, dangerous or inaccessible to experiments. Computational Science and Engineering (CSE) is a rapidly growing interdisciplinary area connecting science, engineering, mathematics and computer science. However, CSE is different from traditional disciplines. It represents a third way which complements theory and experiment. CSE requires a dedicated educational process to be effective in research, both in academia and industry.

We plan to give an overview of experience and research in CSE with the goal of making this field better known to a broader community. European universities were among the first to establish CSE programs (e.g. KTH Stockholm, ETH Zürich, Erlangen). We want to provide an exchange of information between CSE curricula in Europe and elsewhere. Two CSE graduates will present research papers.

State-of-the-art and future research directions in computational electromagnetics. **Thomas Weiland** (TU Darmstadt, Germany) IC/MT2652/010

Computational Electromagnetics has become an integral part of virtually every design process in industry and research in almost every application area of electromagnetic fields. The reliability of todays software tools has grown to a stage which allows solving for larger and larger problems with 10**9 to 10**10 unknowns. With the shear size of these new classes of problems completely new classes of problems appear as well. Handling the plain input data set becomes a crucial issue. Geometrical object descriptions with 100.000 polygonal elements create a new complexity which can no longer be e treated by a person sitting at a screen inspecting the structure to be solved. Time domain simulations may create 10**12 to 10**14 double precision numbers as a typical result. Thus dedicated methods have to be developed for dealing with such massive amounts of data. The tremendous progress in research over the last three decades has created a large variety of reliable algorithms for very realistic applications. Today we are entering a transition period where there is a wide choice of possible algorithms for any given problem. Thus a methodology will be developed to automatically choose the most appropriate solution for a specific task.

Student Talk (15 mins.): *Comparison of hybrid methods for numerical prediction of aeroacoustic noise.* **Claudia Guenther** (RWTH Aachen, Germany), Michael Rom (RWTH Aachen, Germany), Thomas Gotzen (RWTH Aachen, Germany) IC/MT4784/140

In the recent years the emitted sound by aircraft has become a very contributing fact during the development process. Windtunnel experiments, however, are very expensive and so is also the direct computation of noise by solving full 3D Navier-Stokes equations.

The current study investigates various aspects of the hybrid approach via large-eddy simulation (LES) and different computational aeroacoustics (CAA) methods, such as the Ffowcs-Williams-Hawkings equation (FWH) with acoustic-pertubation-equations (APE).

That is, an interface between the LES and CAA solvers will be implemented to find an optimal balance for the three computational domains, the acoustic source region, the near field and the far field, in terms of computational efficiency and accuracy. A detailed analysis of spatial resolution of the acoustic source region and its impact on the acoustic field will be performed to acquire insight into the jet noise physics.

Student Talk (15 mins.): *Numerical simulations of fluid-structure-acoustic interactions to analyze human voice generation.* **Markus Gebhard** (Universität Erlangen-Nürnberg, Germany) IC/MT4914/140

After a larynx excision, as consequence of e.g., laryngeal cancer, the base of the human voice gets lost and a substitute voice is needed to communicate. A possible base of such a substitute voice represents the upper part of the esophagus, called the pharyngeal-esophageal (PE) segment. Via a valve, which the surgeon places between the esophagus and the trachea, the patient can guide air from the trachea into the esophagus. By virtue of that air stream the PE segment starts to vibrate and sound is generated, which can be used as base of a substitute voice. The future goal is to optimize the form of the PE-Segment, in order to ease and improve the artificial voice generation, by the use of simulations.

This substitute voice thereby consists out of three sources:

- the mechanical induced;

- the fluid mechanical induced; and
- the modulated sound sources.

The theoretical base of the stream-noise is represented by Lighthills analogy. Within the author's Master-thesis the research FEM-code CFS++ has been extended to fully coupled Fluid-Structure–Acoustic interactions in a single iterative staggered code.

Computational science education in the United States. **Michael Mascagni** (Florida State University, USA) IC/MT3845/140

We will examine several different types of computational science programs in the United States. We will give examples of undergraduate and graduate programs and attempt to classify the types of educational offerings currently available in the United States. At present many different types of US institutions are offering degree and non-degree programs in Computational Science. We will present examples of several types of these offerings.

CSE programs in Europe. **Lennart Edsberg** (Kungliga Tekniska högskolan, Sweden) IC/MT3278/010

In Europe CSE programs have been given for ten years. In 1997 the following three European universities offered Master programs in CSE: KTH (Stockholm), ETH (Zuerich) and University of Erlangen-Nuernberg. Since then there has been an increasing interest in this interdisciplinary science beacuse of its importance of making high performance computer simulations in e.g. fluid dynamics, electromagnetics, material science, quantum chemistry, molecular dynamics, biosciences, etc.

Today the number of European CSE programs has increased to more than 20 leading to a MSc and about 5 leading to BSc. It is desirable not only to start up more programs for the increasing demand of students with CSE education from applied sciences and industry. It is also important to initiate networks and other fora for presentation and exchange of teaching experience and successful curricula in this educational process.

In this talk an overview is given of the development of CSE programs in Europe so far. Examples of different syllabi and ways of organizing programs will be given as well as a discussion of further developing possibilities and improvements in the future.

IC/MP67/010: Computational science and engineering (CSE). #2

Organiser: Kaspar Nipp (ETH Zürich, Switzerland)
Co-organiser: Hans-Joachim Bungartz (TU München, Germany)
Co-organiser: Oskar von Stryk (TU Darmstadt, Germany)

(For abstract, see session #1 above.)

CSE/CE programs in Germany. **Oskar von Stryk** (TU Darmstadt, Germany) IC/MT2756/010

In recent years a remarkable number of cross-disciplinary study programs with graduate and undergraduate degrees in Computational Science and Engineering/Computational Engineering have been introduced at German universities. Similarities and differences in their curricula, educational goals and formal organization as well will be discussed. Conclusions on the further development on these programs will be drawn.

How to teach CSE?. **Hans-Joachim Bungartz** (TU München, Germany) IC/MT2996/010

Due to the interdisciplinary character of Computational Science and Engineering (CSE), each respective curriculum will contain contents and complete modules or courses from applied mathematics, informatics, and some field(s) of application such as physics or fluid mechanics. However, a serious education in CSE must go beyond a mere building block strategy. The CSE-specific core knowledge and skills to be imparted have to be identified, and innovative arrangements of topics as well as formats for courses are essential for a study program tailored to the needs of computational scientists and engineers in academia and industry.

This contribution will deal with some general educational aspects of study programs in CSE and report experiences with software group projects from the CSE master's program at TUM and from the Bavarian Graduate School of Computational Engineering, an honours program within the Elite Network of Bavaria.

Panel discussion (1 hour): *CSE has landed: who will give it a home and budget?.* **Kaspar Nipp** (ETH Zürich, Switzerland) IC/MT3763/140

In recent years, an increasing number of universities, especially those representing the engineering and natural sciences, have established study programs or research centers for CSE.

As a young and cross-disciplinary field, CSE needs special care and support concerning both research and education. After the different presentations, each focusing on a specific CSE-related aspect, the panel discussion concludes our minisymposium on CSE and, in particular, addresses the following questions:

- Why do we need CSE research and education?
- Should CSE education be implemented as a minor within existing related study programs (such as mathematics, computer science, physics, a classical engineering or science program) or should it be established as a major? If so, on a master's level only or also as an undergraduate program?
- Which departments are best suited to host CSE programs? Or do we need a new departmental structure (real or virtual) reflecting the cross-disciplinary character of CSE?
- The funding agencies are typically organized following the classical university subjects. Can this structure ensure an appropriate reviewing process and, hence, the funding CSE deserves and needs?

We expect a lively discussion and strongly encourage interaction with the audience.

IC/MP475/010: Computational science: teaching and textbooks.

Organiser: Gilbert Strang (Massachusetts Institute of Technology, USA)

An important responsibility of the computational science community is education of the next generation (and the present one!). This minisymposium will discuss essential goals in teaching scientists and engineers and mathematicians. In most cases their courses will combine science and algorithms and software—and we have work to do in finding the right combination and a successful approach.

The minisymposium is open to ideas from all participants at ICIAM.

Teaching computational science with computer algebra. **Walter Gander** (ETH Zürich, Switzerland) IC/MT3692/140

Modern powerful laptops equipped with a computer algebra system offer new ways to teach algorithms that are used in computational science. In this talk we discuss several examples. We show that by including computer algebra the students can concentrate more on fundamentals than on tedious details which sometimes obscure the goals.

Computer science for scientific computing. **G Stewart** (Univ. Maryland at College Park, USA) IC/MT3693/140

The AMSC program at the University of Maryland is an interdisciplinary program offering advanced degrees in applied mathematics and scientific computing. Most of our students have undergraduate degrees in mathematics, science, or engineering. Although these students are often fine programmers, few have had any systematic exposure to computer science. To remedy this lack, we have instituted a course that surveys topics in computer science: computer architecture, languages, compilers, run time environments, parallel computing, and networking. I have taught this course three times and am currently preparing a book "Computer Science for Scientific Computing" to support the course. In this talk I will share my teaching and writing experiences and perhaps draw a few conclusions.

A course in computational science and engineering. **Gilbert Strang** (Massachusetts Institute of Technology, USA) IC/MT487/010

Over the past 20 years we have developed a course that combines applied mathematics with scientific computing. Each lecture and each section of the text discusses a model problem and a code to solve it. The course is popular with engineering students and their departments who want exposure to ideas and also to software (especially MATLAB).

The main sections of the course are Applied Linear Algebra, Differential Equations, Finite Differences and Finite Elements, Fourier Methods, Analytical Methods, Large Sparse Systems, and Optimization. The starting point is to understand the second difference matrices that appear everywhere in scientific computing and simulation.

The need to move beyond the older courses in engineering mathematics, and make the connections with computing, is widely recognized. A pure software course misses the foundations for understanding new problems. The combination of analysis and computational engineering is powerful.

Lessons from Oxford's problem-solving squad. **Lloyd Trefethen** (University of Oxford, UK) IC/MT3691/140

In their first term, first-year DPhil students in Numerical Analysis at Oxford participate in the "Problem Solving Squad". Each week for six weeks, working in pairs, they tackle a computational problem whose answer is a single real number, and the aim is to find a solution numerically to high accuracy – ideally ten digits. I will mention some recent problems we have particularly enjoyed and comment on some lessons learned along the way.

IC/MP4330/010: Numerical computation using portable, extensible toolkit for scientific computation (PETSc).

Organiser: Hong Zhang (Argonne National Laboratory, USA)

Portable, Extensible Toolkit for Scientific Computation (PETSc) is a suite of data structures and routines for the scalable (parallel) solution of scientific applications modeled by partial differential equations. This minisymposium aims at the people engaged in algorithmic research and software development on large-scale numerical simulations. It provides opportunity for the current PETSc users to present their applications and their requirements for the future, as well as introduces potential users on how the software tools can be used to ease the difficulty and reduce the development time on their complex mathematical problems. This is also a good occasion for informal exchanges and discussions between users and developers of PETSc.

Future directions in PETSc. **Matthew Knepley** (Argonne National Laboratory, USA), Dmitry Karpeev (Argonne National Laboratory, USA) IC/MT4337/140

A major thrust of new PETSc development is the incorporation of a general framework for computational meshes and functions defined over them. Building on the Sieve abstraction for topology management, the new Mesh and Section classes allow unstructured mesh handling mirroring the existing DA class. We have also begun to integrate these into the DMMG multigrid framework. Example problems in PETSc will be shown and discussed.

Experiences on solving multi-physics problems with PETSc. **Xiao-Chuan Cai** (University of Colorado at Boulder, USA) IC/MT4338/140

Domain decomposition methods have been well studied for linear and nonlinear elliptic type problems. In this talk, we discuss some recent experimental work on using domain decomposition methods to some harder problems arising from multi-physics simulations, such as magnetodydrodynamics, boundary control of Navier-Stokes equations, and parameter identification problems. We present results based on a PETSc implementation of the Newton–Krylov–Schwarz methods and the focus is on the scalability of the methods when the number of processors is large.

Solving surface motion driven by surface diffusion with PETSc. **Wen Zhang** (Oakland University, USA), Ian Gladwell (Southern Methodist University, USA) IC/MT4341/140

We analyze the performance of the method of lines when solving a fourth order nonlinear partial differential equation with a moving boundary describing microstructural evolution of particles in a sintering process. Both the sequential ordinary differential equation solver and the corresponding parallel ordinary differential equation solver in PETSc are used in the study. We compare and discuss the performance and results.

Optimization of data-access delay. **Xian-He Sun** (Illinois Institute of Technology, USA) IC/MT4689/140

Although rapid advances in computing technology are bringing Petaflop systems within grasp, developing software on high end computers seems more elusive than that of ten years ago. The most significant question of computing remains the same today as it has been for decades: How can software applications take advantage of hardware computing power?

In this talk, I will describe the issues of performance evaluation, measurement, and optimization of high end systems, with a focus on sparse numerical computation. Existing metrics and methods will be summarized, and new challenges will be discussed. Particularly our recent results on reducing and masking data access delay will be presented, which includes the memory-LogP model for performance evaluation of advanced hierarchical memory system and the aggressive push-model methodology for data prefetching. Experimental results will be used to illustrate the practical impact of the current findings.

IC/MP4330/010: Numerical computation using portable, extensible toolkit for scientific computation (PETSc). #2

Organiser: Hong Zhang (Argonne National Laboratory, USA)

(For abstract, see session #1 above.)

Recent additions to PETSc, the scalable library for eigenvalue-problem computations. **José Román** (Universidad Politecnica de Valencia, Spain) IC/MT4349/140

SLEPc, the Scalable Library for Eigenvalue Problem Computations, is a software library for the solution of large, sparse eigenvalue problems on parallel computers. It can be used for the solution of problems formulated in either standard or generalized form, both Hermitian and non-Hermitian, with either real or complex arithmetic, as well as other related problems such as the singular value decomposition.

SLEPc focuses on sparse problems, for example, those arising after the discretization of partial differential equations. Several eigensolvers are available, such as Krylov–Schur, Lanczos, Arnoldi, Subspace Iteration and Power/RQI. SLEPc also provides built-in support for different types of problems and spectral transformations such as shift-and-invert or spectrum folding.

SLEPc is built on top of PETSc and extends it with all the functionality necessary for the solution of eigenvalue problems. This talk focuses on the features that have been added in the last year of development. The main additions are:

- A new eigensolver based on the Krylov–Schur method. This solver can be used for both symmetric and non-symmetric problems, and incorporates an effective restarting mechanism that makes it competitive with ARPACK.
- A new module for computing the truncated singular value decomposition (SVD) of a large sparse rectangular matrix, either via an eigensolver or by means of a specific algorithm such as Lanczos bidiagonalization.

SLEPc website: http://www.grycap.upv.es/slepc/.

Shift-and-invert parallel spectral transformations (SIPs) for solving eigenvalue problems. **Hong Zhang** (Argonne National Laboratory, USA) IC/MT4336/140

SIPs is a new efficient and robust software package implementing multiple shift-and-invert spectral transformations on parallel computers. Built on top of SLEPc and PETSc, it can compute very large numbers of eigenpairs for sparse symmetric generalized eigenvalue problems. The development of SIPs is motivated by applications in nanoscale materials modeling, in which the growing size of the matrices and the pathological eigenvalue distribution challenge the efficiency and robustness of the solver.

In this talk, I will present a parallel eigenvalue algorithm based on distributed spectrum slicing, describe the object-oriented design and implementation techniques in SIPs. As a PETSc developer, I will use this work as an example to illustrate how to efficiently develop special-purpose application code on the top of available parallel software packages.

Solving generalized complex-symmetric eigenvalue problems arising from resonant MEMS simulations with PETSc. **Tsuyoshi Koyama** (ETH Zürich, Switzerland), Sanjay Govindjee (ETH Zürich, Switzerland) IC/MT4832/140

In the operation of high frequency resonators in micro electromechanical systems(MEMS), there is a strong need to be able to accurately determine the energy loss rates or alternatively the quality of resonance. The resonance quality is directly related to a designers ability to assemble a high fidelity system response for signal filtering, for example. This has implications on robustness and quality of electronic communication and also strongly influences overall rates of power consumption in such devices - i.e. battery life. An index of the quality of resonance Q is inversely proportional to the amount of energy loss existing in the system, and can be defined in terms of the complex-valued eigenvalues ω of the system as, $Q = \frac{\mathrm{Abs}[\omega]}{\mathrm{Im}[\omega]}$. In this presentation, we examine methods for accurately simulating energy loss using the direct modeling of acoustic radiation via perfectly matched layer (PML) technology for 3-D structures, which results in complex-symmetric mass and stiffness matrices. Thus it is crucial that one is able to accurately compute eigenvalues of a complex-symmetric system. 3-D modeling increases the number of degrees of freedom and complexity in obtaining the solution, resulting in a requirement for more computing power and memory which can only be supplied by parallel computing methods. The simulations are conducted through the MEMS simulation software HiQLab in combination with the parallel numerical library PETSc. Different methods for preconditioning the iterative solution of linear systems of equations, a required step in the eigensolve, are pursued.

IC/MP123/145: Computational methods in astrophysics and cosmology.

Organiser: Wesley Petersen (ETH Zürich, Switzerland)
Co-organiser: George Lake (Universität Zürich, Switzerland)

Numerical simulations of N-body systems began with $O(N^2)$ methods which computed the force on particle j via

$$\mathbf{F}_j = G \sum_{i \neq j}^{N} m_j m_i (\mathbf{x}_j - \mathbf{x}_i)/|x_j - x_i|^3$$

which for millions of objects quickly became prohibitive computationally. In consequence, tree, particle-in-cell, and adaptive methods have been developed. Adding gas and other energy forms to the simulations requires more sophistication. In planetary system formation problems, a very large number of timesteps are also required. In this minisymposium, various techniques and computational experiences will be discussed.

Parallel Particle Based Simulations in Astrophysics. **George Lake** (Universität Zürich, Switzerland) IC/MT3969/145

I will describe the issue and methods that we use for problems from planet formation to cosmology. These are all spatially and temporally adaptive and based on particle methods. The range of codes are gravitation, SPH (Smooth Particle Hydro) and "rock/sand" dynamics with surface friction. Results will focus on the evolution of dark matter in the current cosmological model. We have used a variety of parallel machines over the years and are now getting interested in various accelerators from CELLs to GPUs.

Asymptotics of expanding cosmological models. **Alan Rendall** (Max-Planck-Institut Potsdam, Germany) IC/MT3973/145

Cosmology describes the universe on the largest scales which can be observed and there the dominant physical force is gravity. The appropriate description of gravity in this context is given by general relativity, where the Einstein equations are coupled to equations describing matter. The realization in the last decade that the expansion of the universe is accelerated has led to the consideration of exotic types of matter with negative pressure. This talk will describe mathematical results on the dynamics of solutions of the Einstein equations coupled to matter, conventional or exotic. In particular it will explain some of what is known about the asymptotics of a phase of unending cosmological expansion.

Stability of solutions to the Einstein equations: Cauchy problem for the Einstein vacuum equations with asymptotically-flat initial data. **Lydia Bieri** (ETH Zürich, Switzerland) IC/MT3990/145

Gravity within General Relativity (GR) is described by spacetime curvature. And the Einstein equations link the curvature of the spacetime to its matter content. For many physical situations, it is appropriate to study the Einstein equations in vacuum (EV). To describe isolated gravitating systems within GR, we consider asymptotically flat solutions of these equations. Examples for such isolated gravitating systems are binary stars, clusters of stars, galaxies etc. They all have in common, that they can be thought of as having an asymptotically flat region outside the support of the matter. This talk shall focus on the Cauchy problem for the EV equations and discuss asymptotically flat solutions of these equations. It will explain some completeness results in view of these solutions.

Numerical models for cosmic-ray modified hydrodynamics. **Francesco Miniati** (ETH Zürich, Switzerland) IC/MT4051/145

Astrophysical flows are commonly turbulent and supersonic, be it on planetary, galactic or cosmic scales. Dissipation mechanisms, particularly at shock waves, are regulated by particle wave interactions in addition to viscous effects, giving rise to populations of suprathermal (cosmic-rays) particles that are dynamically important. After discussing the microscopic issues involved in a correct solution of the problem, I will describe a numerical model, based on Glimm's method and a modified Riemann's solver, for a fluid system made of gas and cosmic-ray particles. I will present test results and discuss current issues and future developments of the presented method.

IC/MP123/145: Computational methods in astrophysics and cosmology. #2

Organiser: Wesley Petersen (ETH Zürich, Switzerland)
Co-organiser: George Lake (Universität Zürich, Switzerland)

(For abstract, see session #1 above.)

Supersonic turbulence in shock bound slabs . **Doris Folini** (ETH Zürich, Switzerland), Randall LeVeque (University of Washington, USA), Rolf Walder (ETH Zürich, Switzerland), Jean Favre (CSCS, Manno, Switzerland) IC/MT4085/145

Supersonic turbulence is a main agent for structure formation in space, from stellar winds to wind-blown bubbles, supernovae remnants, and the interstellar medium. Dissipation is mostly due to shocks. Under isothermal conditions, density is log-normally distributed, with a variance that grows with Mach number, the exact scaling of which is under debate. We discuss 2D and 3D numerical simulation of supersonic turbulence in plan-parallel slabs. We present scaling laws derived from dimensional analysis of the problem. Simulations provide scaling parameters, give a deeper insight into the dissipation mechanism, and provide high-order structure functions which are observable in space.

Low Mach-number models in computational astrophysics. **John Bell** (Lawrence Berkeley National Laboratory, USA) IC/MT4107/145

The early stages of a type-Ia supernova are characterized by long periods of convection leading up to ignition and propagation of deflagration waves. Both the convection and the deflagration waves are low Mach number flows. In this talk, we will introduce numerical models for the simulation of Type-Ia supernovae based on a low Mach number formulation. The low Mach number formulation analytically removes acoustic wave propagation while retaining the compressibility effects resulting from nuclear burning and ambient stratification. This formulation generalizes low Mach number models used in combustion that are based on an ideal gas approximation to arbitrary equations of state such as those describing the degenerate matter found in stellar material. The low Mach number formulation permits time steps that are controlled by the advective time scales resulting in a substantial improvement in computational efficiency compared to a compressible formulation. We will briefly discuss the basic discretization methodology for the low Mach number equations and their implementation in an adaptive projection framework. Computational results illustrating application of the methodology will be presented.

On the cusp of the dark matter. **Hugh Couchman** (McMaster University, Canada) IC/MT4211/145

The Lambda Cold Dark Matter model, now strongly constrained by direct observation at early epochs, successfully describes the structure of the evolved universe on large and intermediate scales. Among the significant problems is a persistent discrepancy between observations of nearby galaxies, which imply that galactic dark matter haloes have flat cores, and the cosmological model, which predicts that the halo should have a central density cusp. Using N-body simulations with star formation and feedback we show that random bulk gas motions in small primordial galaxies, of the magnitude expected in these systems, result in a flattening of the central dark matter cusp on short timescales. Gas bulk motions in early galaxies are driven by supernova explosions and stellar winds from ongoing star formation. During the subsequent evolution, most of the galactic gas will be consumed by star formation and lost via galactic winds, leaving a gas content in agreement with obser-

vations of present-day galaxies. The mechanism is general and would have operated in all star-forming galaxies at redshifts > 10. Once removed, the cusp cannot be reintroduced during the subsequent merger hierarchy involved in building larger galaxies. As a consequence, in the present universe both large and small galaxies would have flat dark matter core density profiles, in agreement with observations.

IC/MP687/015: Geometric-topological methods for 3D shape classification and matching.

Organiser: Michela Spagnuolo (Consiglio Nazionale delle Ricerche, Italy)

The volume and type of information made available via the web is increasing at an extraordinary speed and search engines have become the preferred interaction tools for engaging with this data deluge. In particular, search and retrieval of three-dimensional media will rapidly become a key issue in the upcoming panorama of multimedia content: 3D is indeed expected to represent a huge amount of traffic and data stored in the Internet. 3D media, or shapes, are digital representations of either physically existing objects or virtual objects that can be processed by computer applications and are primarily characterised by their form or spatial extent in the 3D space.

The problem of shape classification and matching is traditionally approached by finding effective abstract descriptions for shapes and by defining efficient methods to estimate the similarity among them, via the computation of some distance measure among descriptors.

In this context, the programme of minisymposium will provide an overview of recent advances in the area, focusing on descriptors as well as on methods to use them for retrieval and classification. The first part, more oriented towards shape descriptors, will cover approaches based on the exploitation of geometric properties as well as approaches oriented to the characterization of the shape topology, up to the very recent advances related to the use of eigenfunctions of the Laplace-Beltrami operator to characterize a shape in an intrinsic manner.

The second part, more oriented towards the use of descriptors to evaluate the similarity among shapes, will cover approaches based on partial and global graph-matching techniques and combinations of different techniques to support the classification process. An analysis of open problems and future perspectives will conclude the programme.

Laplacian eigenfunctions for shape matching. **Bruno Levy** (INRIA Lorraine, France) IC/MT2919/147

In 3D geometry processing, classifying and matching shapes is of paramount importance. With the advance of 3D scanning technology, it is now reasonably easy to create large geometric databases, as done for instance in the AIM@SHAPE European project (see http://shapes.aim-at-shape.net/index.php).

To make an efficient use of this data, classifying and matching meshes has became an important issue in geometry processing. In this context, one of the important problems concerns the matching between two different meshes representing the same object (or two objects with similar shapes).

To efficiently transfer informations (e.g. textures) between those two meshes (or to determine these two meshes as two instances of the same object), one needs to find shape descriptors that are independent on the discretization of the object.

Another way of thinking about the problem is to think in terms of coordinates and parameterization. In this talk, we investigate the use of Laplacian eigenfunctions to define such coordinates. In our talk, we will review the state of the art, and propose new directions of research.

Matching shape graphs. **Fatih Demirci** (Universiteit Utrecht, The Netherlands) IC/MT3396/147

With ever growing databases containing multimedia data, indexing has become a necessity to avoid a linear search. We propose a novel technique for indexing multimedia databases whose entries can be represented as graph structures.

In our method, the topological structure of a graph as well as that of its subgraphs are represented as vectors in which the components correspond to the sorted Laplacian eigenvalues of the graph or subgraphs. Instead of using the adjacency matrix for graph characterization as done in some earlier work, we characterize our graphs based on the Laplacian spectrum, which is more natural, more important, and more informative about the input graphs.

We draw from recently-developed techniques in the field of spectral integral variation to overcome the problem of computing the Laplacian spectrum for every subgraph individually. We will discuss techniques to reduce the cost we pay for computing such a signature.

Having established the signatures, the indexing now amounts to a nearest neighbor search in a model database. By doing such search around the query spectra, similar but not necessarily isomorphic graphs are retrieved. Given a query graph, a voting schema ranks database graphs into an indexing hypothesis to which a final matching process can be applied. The novelties of the proposed method come from the powerful representation of the graph topology and successfully adopting the concept of spectral integral variation in an indexing algorithm. To examine the fitness of the new indexing framework, we have performed a number of experiments using an extensive set of recognition trials in the domain of 2-D and 3-D shape recognition. The experiments, including a comparison with a competing indexing method using two different graph-based object representations, demonstrate both the robustness and efficacy of the overall approach.

Shape-matching and classification using structural descriptors. **Simone Marini** (Consiglio Nazionale delle Ricerche, Italy) IC/MT2503/147

Technological improvements related to object acquisition, visualization and modeling, have caused a considerable growth of the number of 3D models in digital form. Digital 3D models are now available in large databases of shapes, ranging from unstructured repositories, like the web, to specialized catalogues used in engineering and simulation. In this panorama it is clear that methods for the retrieval and automatic classification of 3D content will play a crucial role in the development of efficient applications for the organisation and filtering of 3D data.

The use of structural descriptors is an intermediate step between the geometry and the semantics of the object. Structural descriptors characterize features of the object that are relevant to the application context the matching process is focused on. Moreover information about the shape structure may make the difference when the sub-part analysis supports the automatic classification and/or retrieval processes.

Starting from these remarks, the application of a methodology based on the coupling of geometric and structural information will be discussed for the global and partial matching of 3D shapes and for their automatic calssification.

Future perspectives in shape classification and matching: the role of semantics in similarity assessment. **Bianca Falcidieno** (Consiglio Nazionale delle Ricerche, Italy) IC/MT2531/147

It is quite evident that reasoning about shapes naturally leads to refer to resemblance, similarity, or equivalence concepts, which are the basis for shape description and retrieval. Current approaches to these problems involve complicate geometric comparisons and, despite the recent improvements, all development has focused on geometry, which provides a complete description of the (geometric) shape of a solid. The choice of a mathematical model is mainly determined by a set of restrictive computational requirements such as representational finiteness, constructivity and completeness, which are related to the properties of the mathematical model.

But it also should consider other constraints imposed by downstream applications. When we want to portray the complexity of nature or intricate man-made objects, traditional geometric entities are unable to do so in a manageable and controllable fashion. The result is that information related to the meaning or function of an object is something *attached* to its geometry if not an alternative to it. Current systems are unable to measure similarity according to criteria relevant for specific application domains, such as manufacturing or product modelling. Therefore, it is important to develop ways to measure similarity among shapes, that can tell us how similar or different they are in a specific context and that reflect those notions of similarity useful in the application context in which it has to be used.

In this scenario, it is interesting and challanging to reformulate the traditional modelling paradigm by formalising the concept of *meaning*, through the definition of a semantic universe in addition to the physical one. This means building a conceptual model of the application domain based on a set of fundamental classes or types. In addition to the physical universe related to the real or virtual world, a semantic universe could be defined for representing human knowledge of a particular domain.

IC/MP687/015: Geometric-topological methods for 3D shape classification and matching. #2

Organiser: Michela Spagnuolo (Consiglio Nazionale delle Ricerche, Italy)

(For abstract, see session #1 above.)

Mathematical tools for shape classification and matching. **Michela Spagnuolo** (Consiglio Nazionale delle Ricerche, Italy) IC/MT2038/147

While information is moving from textual to visual form, supported by emerging technologies, *digital shapes* are becoming more and more important. Digital shapes populate virtual environments in advanced scientific simulation as well as in emerging edutainment applications.

Due to the recent improvements the acquisition, visualization and modeling technologies, the number of 3D shapes available on the web is more and more growing, and there is an increasing demand for tools supporting the automatic search for 3D objects and their sub-parts in digital archives.

Assessing the similarity among 3D shapes is a very complex and challenging research topic. While human perception have been widely studied and produced theories that received a large consensus, the computational aspects of 3D shape retrieval and matching have been only recently addressed.

This has also caused a gradual shift of research interests from methods to represent shapes towards methods to *describe* shapes in Computer Graphics as well. This has led to a rapidly increasing number of methods and tools addressing the same basic issues targeted by Computer Vision, that is, segmentation, recognition and understanding. While a digital model, either pixel- or vector-based, is a digital representation which is quantitatively similar to an object, its description is only qualitatively similar.

Shape analysis and understanding are therefore basic tools for constructing object descriptions, necessary to answer problems arising in the many applications which deal with digital shapes.

Differential topology methods for shape description. **Silvia Biasotti** (Consiglio Nazionale delle Ricerche, Italy), Daniela Giorgi (Consiglio Nazionale delle Ricerche, Italy), Giuseppe Patanè (Consiglio Nazionale delle Ricerche, Italy) IC/MT2443/147

Differential topology, and specifically Morse theory, provides a suitable setting for formalizing and solving several problems related to shapes analysis. The fundamental idea behind Morse theory is that of combining the topological exploration of a shape with quantitative measurement of geometrical properties provided by a real function defined on the shape.

Several functions (e.g. harmonic fields and laplacian eigenfunctions) have been studied in contexts such as shape abstraction, parameterization, and comparison. Each of them gives a measure of specific properties of the input shape, playing the role of the *lens* through which we look at the properties of the shape. To compare the information provided by these functions, we analyse methods which use the configuration of isocontours and critical points for encoding 3D shapes, e. g. Reeb graphs.

Geometrical shape comparison by size theory. **Patrizio Frosini** (Università di Bologna, Italy) IC/MT2565/147

Size Theory allows us to compare shapes of topological spaces and manifolds with respect to properties described by real functions. The main tools used in Size Theory are some pseudodistances measuring the minimal changes of these real functions under the action of homeomorphisms. This leads to considering *size pairs* (S, f), where S is a topological space and f is a continuous *measuring function* with real values. For example, the different "bumpiness" of two closed surfaces X, Y in the Euclidean space can be compared by considering two manifolds $S(X) := X \times X$, $S(Y) := Y \times Y$ and taking the functions defined by setting $f_X(P_1, P_2) = -\|P_1 - P_2\|^2$, $f_Y(Q_1, Q_2) = -\|Q_1 - Q_2\|^2$.

When two shapes must be compared according to a new comparison criterion, the first step is to find the "right" set of corresponding properties, i.e. of size pairs $(S(X), f_X)$, $(S(Y), f_Y)$. The next step in the comparison process is to consider the *natural pseudo-distance*

$$d((S(X), f_X), (S(Y), f_Y)) := \inf_{h \in H} \sup_{P \in S(X)} |f_X(P) - f_Y(h(P))|,$$

where h varies in the set H of all homeomorphisms between $S(X)$ and $S(Y)$.

In this way, two objects are judged to be sharing the same shape if and only if they share the same shape properties; i.e., the natural pseudo-distance between the associated size pairs vanishes. This method can be adapted to several different definitions of shape without changing its geometrical-topological framework. Some new results about this approach to shape comparison are illustrated.

Deformation invariant 3D model descriptors. **Dietmar Saupe** (Universität Konstanz, Germany) IC/MT3814/147

In content-based 3D model retrieval the most commonly adopted approach is based on feature vectors that capture characteristics of corresponding surfaces. A suitable metric in feature vector space allows searching for the nearest neighbors of a query object. The feature vectors are typically designed with the goal of invariance with respect to scale and rigid object motion. However, in applications one may also wish to retrieve objects similar to the query object allowing certain nonlinear deformations. For example, one my wish to find objects with the same topological structure, that may be given by a graph connecting critical points of a suitable Morse function on the surface. Alternatively, one has considered invariance with respect to isometric transformations, i.e., deformations that do not stretch or tear the surface. In this presentation we briefly survey the approaches for 3D object retrieval with topological and bending invariance. A problem with the retrieval of isometric surfaces is the inherent complexity of the search that boils down to general graph matching known to be NP-hard. In our work we propose a statistical descriptor that provides a faster match but may not provide the optimal match between given surfaces. This work was carried out jointly with Mauro Ruggeri.

IC/MP727/015: Level-set methods: fluid applications.

Organiser: Yen-Hsi Tsai (University of Texas at Austin, USA)
Co-organiser: Frédéric Gibou (UC Santa Barbara, USA)
Co-organiser: Stanley Osher (University of California, Los Angeles, USA)

Several problems that arise in science and engineering can be formulated as a front evolution between two (or more) phases. Examples include solidification problems, dendritic growth in materials science, free surface flows, multiphase flows, to cite a few. One of the main the difficulties in solving such problems comes from the fact that the interface location must be computed as part of the solution to the underlying equations. Since their inception, level set methods have been extremely successful in tackling these problems. In this minisymposium, the focus will be given In this minisymposium the focus will be given to recent advances in the core level set algorithms as well as their applications. Specifically, the core algorithm will cover topics on adaptivity, volume conservation, and solving inverse problems. Applications will include multiphase flows, high frequency wave propagation and shape optimization. This minisymposium will offer an excellent opportunity for researchers to learn about a wide variety of recent developments in the computational aspects of level set methods as well as their applications and will stimulate cross-pollination between disciplines.

A new stability condition for surface tension-driven flows. **Paul Vigneaux** (Université de Bordeaux, France), Cédric Galusinski (Université du Sud-Toulon-Var, France) IC/MT4313/015

We consider models for the simulation of curvature-driven incompressible bifluid flows, where the surface tension term is discretized explicitly. Since Brackbill, Kothe and Zemach (J. Comput. Phys. 100, pp 335-354, 1992) introduced the Continuum Surface Force (CSF) method, many methods involved in interface tracking or capturing are based on this reference work. Particularly, the surface tension term is discretized explicitly and therefore, a stability condition is induced on the computational time step. This constraint on the time step allows the containment of the amplification of capillary waves along the interface, which can be the source of parasitic currents on the interface. The derivation of this stability condition puts more emphasis on the terms linked with the density in the Navier-Stokes equation (i. e. unsteady and inertia terms) rather than on the viscous terms. Indeed, the viscosity does not appear, as a parameter in this stability condition.

In this talk, we propose a new stability condition for which we present a theoretical estimation for flows with low and medium Reynolds numbers. We detail the analysis which is based on a perturbation study - with capillary wave - for which we use energy estimate on the induced perturbed velocity. This stability condition involves the fluid viscosity, emphasizing the role of viscous terms for such flows. We validate and illustrate our analysis with numerical simulations of microfluidic flows using a Level Set method. Finally, we propose a method to reduce computational cost induced by this stability condition for low flow velocities. This method still uses an explicit discretization of the surface tension term and takes advantage, as far as possible, of the stationary behaviour of the interface. This approach was inspired by the simulation of microflows applications which involve the exploration of different mixing regimes inside microdroplets.

Stability of flows in microfluidics. **Thierry Colin** (INRIA Futur Bordeaux, IMB, France) IC/MT4314/015

The aim of this talk is to present some results for interfacial flows in microfluidics. Flows in microfluidics are characterized by low Reynolds numbers and a by the fact that surface tension has a predominant role in stability issues. Jet or co-flows are special configurations that are of great importance for applications. The problem of their stability is therefore central in the understanding of experiments. Our goal is to characterize the stability of a jet of a newtonian fluid into another one when the effects of surface tension and confinement have competitive effects.

We have two different approaches: the first one is to compute directly the solution in a T-junction by a level-set method. This is done in 2-D, 2-D axi and 3-D. The second approach is a numerical spectral analysis: we first linearize the bi-fluids Navier–Stokes equation with free interface and surface tension around a steady-state solution. We then compute numerically the eigenvalues of the linearized operators. The sign of the real part of the eigenvalue gives the stability issue. Moreover, in the case of instability, the wavelength corresponding the the more unstable modes is related to the size of the droplets that are created. We investigate for which regime the jet is stable and we compare the size of the droplets that are created with experimental data.

This is a joint work with C.-H. Bruneau, A. Colin, C. Galusinski, S. Tancogne and P. Vigneaux.

Level-set simulation of solute/solvent interfaces. **Li-Tien Cheng** (University of California, San Diego, USA) IC/MT4138/025

The level-set method of Osher and Sethian for handling interfaces has sparked wide interest in numerous applications, ranging from fluid dynamics to image processing, since its creation. We consider here a level set method with a complicated geometric flow for construction of solute/solvent interfaces.

Investigating spontaneous capillarity-controlled events via the level set method. **Maša Prodanović** (University of Texas at Austin, USA), Steven Bryant (University of Texas at Austin, USA) IC/MT3216/015

An accurate description of the mechanics of pore level displacement of immiscible fluids could significantly improve the macroscopic parameter predictions from pore network models in real porous media. Assuming quasi-static displacement, we describe a simple but robust model based on the level set method for determining critical events for throat drainage and pore imbibition. The method arrives at geometrically correct interfaces while robustly handling topology changes and is independent of the pore space complexity.

IC/MP727/015: Level-set methods: fluid applications. #2

Organiser: Yen-Hsi Tsai (University of Texas at Austin, USA)
Co-organiser: Frédéric Gibou (UC Santa Barbara, USA)
Co-organiser: Stanley Osher (University of California, Los Angeles, USA)

(For abstract, see session #1 above.)

An interface capturing method for two-phase flow with moving contact lines. **Gunilla Kreiss** (Uppsala University, Sweden) IC/MT2883/025

To begin with we discuss a new conservative level set method for immiscible two-phase flow, where each phase is governed by the incompressible Navier-Stokes equation, and the interface is advected with the local velocity. The method is conservative in the following sense: there is a small error in the mass of each the two phases due to the discretization error, but it does not grow over time. In a straightforward application of the method, a no-slip condition is imposed at a solid wall. Thus the resulting model cannot capture contact line dynamics. Inspired by a phasefield method based on Cahn-Hilliard theory for diffuse interfaces, we propose an extended model, which is capable of capturing a moving contact line. This work has been done in collaboration with Elin Olsson, Sara Zahedi, Walter Villanueva and Gustav Amberg.

A field-space-based level-set method for computing multi-valued solutions to Euler–Poisson equations. **Hailiang Liu** (Iowa State University, USA) IC/MT3854/015

We present a field space based level set method for computing multi-valued solutions to one-dimensional Euler–Poisson equations. The system of these equations has many applications, and in particular arises in semiclassical approximations of the Schrödinger-Poisson equation. The proposed approach involves an implicit Eulerian formulation in an augmented space — called field space, which incorporates both velocity and electric fields into the configuration. Both velocity and electric fields are captured through common zeros of two level set functions, which are governed by a field transport equation. Simultaneously we obtain a weighted density f by solving again the field transport equation but with initial density as starting data. The averaged density is then resolved by the integration of the obtained f against the Dirac delta-function of two level set functions in the field space. Moreover, we prove that such obtained averaged density is simply a linear superposition of all multi-valued densities; and the averaged field quantities are weighted superposition of corresponding multi-valued ones. Computational results are presented and compared with some exact solutions which demonstrate the effectiveness of the proposed method.

Solving PDEs on moving interfaces with applications to two-phase flow with surfactants. **Hongkai Zhao** (University of California, Irvine, USA) IC/MT2578/015

I will present an Eulerian formulation for solving PDEs on moving interfaces. In particular we give a decomposition of the surface Laplacian operator which allows us to design a semi-implicit scheme to overcome the stiffness of surface Laplacian operator. Applications to two phase flow with the effects of surfactants will be shown. This is a joint work with J. Xu, Z. Li and J. Lowengrub.

Accurate computation of interfacial, axi-symmetric Stokes flows. **Hector Ceniceros** (University of California, Santa Barbara, USA) IC/MT2771/015

Boundary integral methods have been used widely for the simulation of interfacial Stokes flows. These free surface representations reduce the problem to one defined solely on the fluid interface. However, it is difficult to obtain high order approximations to the resulting line integrals due to their singular nature and intricate structure. Existing quadrature rules for numerical integration of the interfacial velocity are, at best, of a limited second order accuracy. In this work, we analyze the problem of attaining higher order quadratures and propose new numerical approaches to overcome all the difficulties. These approaches are based on an application of analytic and local error corrections constructed from an asymptotic analysis of the integrands. We present quadratures that achieve a uniform accuracy of up to order five and demonstrate their superior accuracy with numerical examples. This is joint work with Monika Nitsche and Aino Karniala.

14: Computational Sciences, Contributed Talks

IC/CTS4647/14: Computer science, software and data-fitting.

Organiser: Walter Krämer (Bergische Universität Wuppertal, Germany)

Bugs, errors, and unexpected results in computer-algebra packages. **Walter Krämer** (Bergische Universität Wuppertal, Germany) IC/CT2336/010

The following is a citation from the Description and aims of of the Dagstuhl Seminar on Algebraic and Numerical Algorithms and Computer-assisted Proofs:

"In contrast, most algorithms in computer algebra are 'never failing', that is they are proved to provide a solution for any input, and the maximum computing time for this is estimated *a priori*.

The focus of the talk will be the reliablity of the computer algebra system Maple. We will show that 'never failing' algorithms may be the theory but concerning actual implementations such a statement seems not to be drawn from life.

Simulation and solution of stochastic systems with a component-based software design. **Martin Krosche** (TU Braunschweig, Germany), Martin Hautefeuille (TU Braunschweig, Germany) IC/CT2435/015

Often uncertainties occur in the numerical simulation of real-world problems. A useful method is stochastic modelling. In this context Monte Carlo (MC) methods and the stochastic Galerkin method are well known and frequently used.

In the field of component-based software systems a component can be seen as an independant software or as a part of a software system. A corresponding architecture allows clearness, flexibility and reusability. The *Component Template Library* (CTL) is a so called middleware to realise component-based software systems, and fits to the requirements of scientific computing.

In this paper we present the design of a software system for the stochastic simulation using MC and stochastic Galerkin methods based on the CTL. For each Stochastic method a number of components are realised to allow parallel features.

Probabilistic model of fuzzy subsets. **Magda Tsintsadze** (Tbilisi State University, Georgia), Tamaz Gachechiladze (Tbilisi State University, Georgia) IC/CT497/015

It's known that except of stochastic uncertainty exists uncertainties of other types, there is an opportunity to expand an area of use for differential equations even in those cases when parameters determining differential equations contain uncertainty of new types and therefore there is no opportunity to pose the classical problem - We are offering modeling of these situations with help of new concept - canonically conjugated fuzzy subset.keywords:Fuzzy sets, Fuzzy Differential Equations, Optimal Membership Functions.

Graphical simulation of a new concept of low sized surgical parallel robot for camera guidance in minimally invasive surgery. **Calin Vaida** (Universitatea Tehnicã Cluj-Napoca, Romania), Doina Liana Pisla (Universitatea Tehnicã Cluj-Napoca, Romania), Nicolae Plitea (Universitatea Tehnicã Cluj-Napoca, Romania) IC/CT811/015

Surgery is one of the fields where robots have been introduced due to their positioning accuracy which exceed the human capabilities. This provided a cure for impossible to treat diseases, but introduced also several drawbacks: high space occupied in the operating room, lack of haptic feedback, extensive training and very high costs. Following a thorough analysis of existing market solutions, the paper presents the graphical simulation of a new concept of modular parallel robot for camera guidance in minimally invasive surgery with several improvements: small occupied volume, a very cheap structure, high reliability, reduced play and a small working volume. In surgery the robot capabilities should not exceed the volume requirements of the operating field, as an erroneous command or an error in the software could cause serious injuries for both patient and medical personnel. A complex simulation program was developed in order to study the geometric, kinematic and dynamic characteristics of parallel robots used for minimally invasive surgery. The facilities of the new achieved simulation software enable the possibility to develop a complex study about the kinematics and dynamics in order to optimize the parallel structure. The simulator is interactively achieved such as the user could influence the simulation parameters and could be informed about the possible errors during the simulation process. This simulation system was conceived to diminish the costs, to reduce the processing time, to optimize the use of the resources during the process implementation or process redesign and to assist specialists for the investments planning. The higher stiffness of the structure used for surgery will ensure a clear and stable image in any extreme position of the robot and the smaller manufacturing costs will make it affordable for a larger number of hospitals and usable in a wider range of interventions allowing more surgeons to get familiar with it.

Optimally scaling particle simulation method using multigrid. **Matthias Bolten** (FZ Jülich, Germany), Godehard Sutmann (FZ Jülich, Germany) IC/CT4798/015

Particle simulation methods are an important tool in different fields of research, e.g. in biophysics or plasma physics. These methods differ in working either directly on the particles or on a meshed representation. Multigrid methods are especially appropriate for the latter and they have been used in different algorithmic implementations. In particle simulation codes based on discrete spacial meshes usually the potential is split into a long-ranged and a short-ranged part. We recently introduced a method using charge-centered B-spline densities for the splitting by rewriting the right hand side of the PDE. As these densities are finitely supported, the resulting complexity is optimal, i.e. of order $\mathcal{O}(N)$. In order to achieve high accuracy, it is favorable to use B-spline densities with large support, even when high-order discretization is used for the solution of the PDE. As a result of this, the resulting complexity is still $\mathcal{O}(N)$, but the prefactor is rather large. Since the splitting formulation results in a convolution of the singular point charges with the B-spline density, Fourier-techniques can be used to sample the point charge replacing densities on the grid. This can be performed most efficiently with a nonequispaced FFT (NFFT), resulting in a large reduction of the prefactor.

In this talk we will present the complete method, which is based on a multigrid solver and which incorporates the NFFT to optimize the preparation step.

IC/CTS4646/14: Chemistry and heat conduction.

Newton–Krylov methods for fully coupling chemistry and transport. **Laila Amir** (INRIA Rocquencourt, France), Michel Kern (INRIA Rocquencourt, France) IC/CT2299/010

Modelling reactive transport in porous media, using a local chemical equilibrium assumption leads to a system of advection-diffusion PDE's coupled with algebraic equations. When several species are transported by a subsurface flow, one of the chemical phenomena involved is sorption, the process by which species may interact with the porous matrix, and become attached to the rock. Solving the chemical equilibrium problem keeps track of how much of the species remain mobile, and how much is fixed.

When solving this coupled system, the algebric equations have to be solved at each grid point for each chemical species and at each time step. This leads to a huge coupled non-linear system.

In this talk, we review different formulations of the coupled reactive transport problem, and we compare a formulation of a proposed global approach with the more tradional operator splitting approach that consists in solving separately the chemical equations and the transport equations. The method is formulated in terms of total mobile and total immobile concentrations. Its main advantage is to keep chemistry distinct from the transport equations, contrary to the more traditional direct substitution approach.

For any realistic configuration, it is not possible to form and store the Jacobian matrix. A better approach is to use Newton-Krylov methods, in which the Jacobian vector product calculated within an iterative Krylov solver may be approximated

instead of being computed with an explicit Jacobian. The product is simply approximated by finite differencing the residual equation in the direction of the Krylov vector.

A critical ingredient needed for the success of a Jacobian-free Newton method is efficient matrix-free preconditioning, since the Jacobian is never computed explicitly. For this purpose, we use an operator-splitting preconditioning which is known to be a good preconditioning technique for this kind of problem.

A regularization approach for surface reconstruction. **Hebert Montegranario** (Universidad de Antioquia, Colombia) IC/CT621/010

Ill-posed inverse problems arise in many branches of science and engineering. In the typical situation one is interested in recovering a whole function given a finite number of noisy measurements on functionals. A regularization approach is one of the solutions for this kind of problem among which we find surface reconstruction from point clouds. In this talk we present a classification of methods for surface reconstruction and its solution in the framework of classical regularization, that is, in terms of linear combinations of the reproducing kernel in certain proper spaces for reconstruction. We evaluate the quality of this solution to approximate 3D data and some examples for computational implementation are also shown in order to complete a user's guide for an efficient employment of kernel methods in the reconstruction of multivariate functions.

Solving multi-subdomains problem in certain nonlinear heat-conduction process. **Antony Siahaan** (University of Greenwich, UK), Choi-Hong Lai (University of Greenwich, UK), Koulis Pericleous (University of Greenwich, UK) IC/CT2471/015

Some coupling techniques for nonoverlapping domain decomposition method are investigated in this paper. We test these methods on some linear and nonlinear heat conduction processes taking place in a multi-chip module which has many geometrically structured subdomains. The problem of interface condition between two adjacent subdomains is tackled by incorporating a defect equation which is solved iteratively. We evaluate two defect equations on this scheme, i.e. the difference of normal derivative and the residual of discretized heat conduction equation itself. Both equations lead to systems of nonlinear equations which are solved by means of quasi-Newton methods with an adaptive alpha rate instead of a Jacobian matrix. The simulation suggests that the second defect equation is much more accurate. The present scheme is also compared with the scheme that uses the Conjugate Gradient method as the nonlinear solver.

IC/CTS4649/14: Fluid dynamics and flows.

Organiser: Stephen Roberts (Australian National University)
Co-organiser: Alicia Guadalupe Ortega Camarena (TU Braunschweig, Germany)

Deterministic sensitivity analysis for a model for flow and transport in porous media. **Estelle Marchand** (INRIA Rocquencourt, France), François Clément (INRIA Rocquencourt, France), Jean Roberts (INRIA Rocquencourt, France), Guillaume Pépin (ANDRA, France), Laurent Loth (ANDRA, France) IC/CT2288/010

The questions of safety and uncertainties are central to feasibility studies for an underground nuclear waste storage site. Uncertainties concerning safety indicators, such as the water flow through outlet channels or the concentrations of contaminants, which are due to uncertainties concerning properties of the subsoil or of the contaminants, must be evaluated.

Probabilistic methods can be used. They give good results and are relatively easy to implement, but they are expensive because they require a large number of simulations. The deterministic methods investigated here are much less demanding in computing time but they give only local information. Thus the two methods are complementary and both deserve to be developed.

The deterministic method used here is based on the singular value decomposition of the Jacobian matrix of the mathematical model of the problem, which consists of a flow equation based on the stationary Darcy law, a transport equation, ie a mass balance equation, for each contaminant, and a law of exchange between liquid and solid phases for each contaminant.

The first step is the computation of the derivatives of the mathematical model. For the flow equation we use a code differentiated through analytical formulas, using the adjoint state method. For the transport equation we combine manual differentiation and automatic differentiation with the library AdolC.

The singular value decomposition provides a hierarchical list of directions in both the space of input parameters and in the space of safety indicators.

For the flow model, various deterministic studies have been computed for a 3 dimensional test case. We observe a weak variability of the local sensitivities when the choice of the input parameters varies in the spectrum of possible input parameters. Probabilistic and deterministic studies provide similar results. We also compare results obtained through a probabilistic and a deterministic analysis for the full model.

COOL: constraints-oriented library. **Ralf Gruber** (École Polytechnique Fédérale de Lausanne, Switzerland), Mejdi Azaiez (Ecole Nationale Supérieure de Bordeaux, France) IC/CT1216/010

The new partial differential equation solver COOL is presented. The solver exactly satisfies external and internal constraints such as $\vec{\nabla}\cdot\vec{u} = 0$ (Stokes, incompressible Navier–Stokes), $\vec{\nabla}\cdot\vec{B} = 0$ (Maxwell), or $\vec{\nabla}\times\vec{E} = 0$(plasma waves). The method is presented by means of the two dimensional Stokes eigenvalue problem in the unit square Ω=$[-1,+1]^2$: *Find* $\vec{u_h} \in \mathbf{X_h}$ *and* $\omega^2 \in \mathbb{R}^+$ *such that*

$$S(\vec{u_h},\vec{v_h}) := \int_\Omega \vec{\nabla}\vec{u_h}\cdot\vec{\nabla}\vec{v_h}\mathrm{d}\mathbf{x} = \omega^2 \int_\Omega \vec{u_h}\cdot\vec{v_h}\, d\mathbf{x},\ \forall \vec{v_h} \in \mathbf{X_h},$$

$$mathbfX_h = \{\vec{v_h}\ ,\ \vec{\nabla}\cdot\vec{v_h} = 0\ ,\ \vec{v_h} = 0 \text{ for } \vec{x} \in \partial\Omega\}.$$

This problem is solved in two steps applying a new constraints oriented non-conforming hp method in which all the terms appearing in the variational formulation have the same functional dependence in each element and the same regularities accross element borders. For this purpose, two canonical polynomial basis functions are defined

$$h_j(x) = -\frac{1}{p(p+1)}\frac{1}{L_p(\xi_j)}\frac{(1-x^2)\,L_p'(x)}{(x-\xi_j)}, \qquad -1 \le x \le +1, \tag{1}$$

$$g_j(x) = h_j(x) - \frac{L_p(x)}{(p+1)L_p(\xi_j)}, \qquad 0 \le j \le p\ ,$$

where L_p is the Legendre polynomial of degree p, L_p' its derivative, and ξ_j, $j = 0,1,..,p$, are the zeros of $(1-x^2)L_p'(x) = 0$. Since $L_p(x)$ is zero at the Gauss points ζ_i, $i = 1,..,p$, $h_j(\zeta_i) = g_j(\zeta_i)$. The function $h_j(x)$ is a polynomial of degree p, continuous accross element borders. It is used to represent partial derivatives that become polynomials of degree $p-1$, discontinuous accross element borders. The function $g_j(x)$ is a polynomial of degree $p-1$, discontinuous accross element borders. It is used to represent terms without deriva-

tives. As a consequence, each term in the variational form and in the $\vec{\nabla}\cdot\vec{u}$ term are polynomials of degree $p-1$ in x and y, discontinuous accross element borders. As a consequence, $\vec{\nabla}\cdot\vec{u}\equiv 0$ can be satisfied. In the first step, $\vec{\nabla}\cdot\vec{u}=0$ is imposed at the Gauss points, leading to algebraic conditions between the old ($\vec{u}$, two components) and the new dependent variables ($\vec{z}$, one component) that remain after elimination of $\vec{\nabla}\cdot\vec{u}=0$. In matrix form these conditions write $\vec{u}=M\vec{z}$. The initial eigenvalue problem $A\vec{u}=\omega^2 B\vec{u}$, issue of eq.(1) then becomes $M^TAM\vec{z}=\omega^2 M^TBM\vec{z}$. The eigensolution of the 2D Stokes spectrum converges exponentially as in conforming hp methods. Only Stokes modes are obtained. The $\vec{\nabla}\cdot\vec{u}=0$ is exactly satisfied. The condition number of the M^TAM matrix is smaller than for a Poisson equation. The matrix M is sparse. Thus, this COOL method is perfect to be applied to time evolutionary problems that are constraint by side conditions such as incompressible Navier–Stokes, or Maxwell's equation.

Finite-volume simulation of inundation due to tsunamis. **Stephen Roberts** (Australian National University) IC/CT2832/144

Hydrodynamic modelling allows flooding, storm-surge and tsunami hazards to be better understood, their impacts to be anticipated and, with appropriate planning, their effects to be mitigated. Geoscience Australia in collaboration with the Mathematical Sciences Institute, Australian National University, is developing a software application called AnuGA, based on the Finite Volume method to model the hydrodynamics of floods, storm surges and tsunami.

In this talk we will describe the computational model used in AnuGA, provide validation of the method using a standard benchmark, and provide the results of a tsunami simulation of the coastal region of north eastern Australia, near the city of Cairns.

Numerical simulation of building evacuation in emergency conditions. **Alicia Guadalupe Ortega Camarena** (TU Braunschweig, Germany) IC/CT2467/015

One of the main contributing factors for human safety regarding on buildings with people inside, is the effective possibility of evacuation after a disaster has occurred. In this sense, different models of human crowds have been developed in order to simulate the behaviour of pedestrians once an emergency condition has occured, and the evacuation of the building is necessary. Simulation models have been conceived from two different perspectives: 1) the psychological scope, and 2) the engineering scope.

Up to now, the two main approaches from the engineering perspective are given by the macroscopic and the microscopic models. One of the first macroscopic-based models are those which approximate the pedestrian movement as a gas or fluid or with particle dynamics, where lattice-Boltzman models, Navier-Stokes traffic-like equations, and H-theorem are the most representatives ones. In the other hand, microscopic-based models take into account the individual characterisitics of the pedestrians, and the crowd-elements are not generalized as it occures in the macroscopic approach. The most representative models are the social force model, and the models based on driving forces created by potential or static/dynamic fields created by the same pedestrians on their way to the emergency exit. For these models the development and the use of cellular automata is frequent. A third new appearing approach is given by the mesoscopic model, which can be seen as an hybrid technique that involves elements of both macro- and micro-scopic approaches, and evenmore some other elements like the virtual reality are also here integrated.

In the psychological perspective, models have been defined by mainly three different concepts: a) what do people see, b) what do people want, and c) what do people perceive from the environment before, during and after an evacuation in an emergency condition. But less in this field has been explored, because of many factors like "lack of knowledge", the almost rare or inexistent information of pedestrian evacuations in real scenarios, which makes the psychological models more vague and intagible.

One of the main objectives in this research is the integration of psychological elements of human behaviour during evacuation, and specially those related to the apparison of panic into our proposed model. Obtaining in this case a more realistic approach of crowd movements during emergency evacuations which later can be used for the evaluation of the influence in the behaviour and dynamics of pedestrians by means of possible physical blockages in the real scenario (e.g. doors, stairs, corridors), and with this to minimize the overall risk of the occupants.

Locally one-directional finite-volume schemes on cubed sphere. **Ramaz Botchorishvili** (Tbilisi State University, Georgia) IC/CT3530/014

An approach for constructing numerical schemes for first order hyperbolic equations on a domain between two spheres will be presented. The approach exploits cartesian data structure of a cubed sphere mesh and operator splitting. Construction of numerical schemes is performed in three steps. First, a semidiscrete scheme is constructed by means of a finite volume method. Then operator splitting is used in a such way that each split equation accounts for one predefined direction only. Finally, an implicit time discretization is done. The resulting fractional step scheme is conservative and stable for large CFL numbers. Numerical results will be presented. Feasibility of the developed approach for some parabolic equations, for a generic PDE solver on a cubed sphere, and for mesh refinement procedures will be briefly discussed.

14: Computational Sciences, Posters

IC/PP4289/015: ***Ab initio* and modeling study of some amino acid-tRNA: NMR shielding and thermodynamic of solvent effect.**

Presenter: Hadieh Monajemi (University of Malaya, Malaysia)
Co-author: W.A.T. Wan Abdullah (University of Malaya, Malaysia)
Co-author: Sharifuddin Zain (University of Malaya, Malaysia)

tRNA takes suitable amino acid to the ribosome for the formation of peptide bonds. In starting a peptide chain, the first amino acid which is taken to the ribosome is methionine. We simulated methionine-amino acid bondings and amino acid-tRNA bondings using mixed study of quantum mechanics ab initio calculation and molecular mechanics. NMR shielding tensors, thermodynamic parameters and total energies have been calculated. It is important to try to answer the question what kind of physical properties and environmental conditions regarding the dipeptides cause tRNA to attach to a wrong amino acid. In fact one of these properties is dielectric, which we calculate its effect.

IC/PP4783/142: The ill-posed retrieval of aerosol extinction coefficient profiles.

Presenter: Pornsarp Pornsawad (Universität Potsdam, Germany)
Co-author: Christine Böckmann (Universität Potsdam, Germany)
Co-author: Christoph Ritter (Alfred Wegener Institute, Germany)
Co-author: Mathias Rafler (Universität Potsdam, Germany)

We regard an ill-posed problem which is ill-posed in the sense that one has to calculate the derivative from noisy data. We prefer to use Tikhonov regularization [1] and a variational method [2] to stabilize the problem. The particular application concerns the retrieval of optical backscatter and extinction coefficient profiles from lidar (*l*ight *d*etection *a*nd *r*anging) signals of aerosol layers in our atmosphere. Since the traditionally used methods show often an unstable behavior we developed and compared three new possibilities. Aerosol extinction and backscatter coefficient profiles were statistically and numerically retrieved from the EARLINET lidar database [3] simulated at the wavelengths 355, 387, 532 and 607 nm with realistic experimental and atmospheric conditions taken into account. Firstly, in using a statistical technique adapted from [4] the density and range corrected signal (RCS) were separately fitted by linear, quadratic and cubic model to avoid an *a priori* assumption on the behaviour of function to be regress. A chi-squared test was used to be the criteria to choose a good fit model for RCS. Secondly, Tikhonov regularization was performed on the calculation of the derivative together with the implementation based on the natural cubic spline. To avoid the task concerning the selection of a suitable regularization parameter and to overcome the instability of traditional methods such as difference methods and interpolation methods, thirdly, a variational method for differentiation was applied. The results were compared with two traditionally used methods. It turns out that all the three developed methods are more accurate than the traditional ones. In spite of the big numerical effort of the variational method it is the most stable one. [1] Wang et al(02) Inverse Problem 18. [2] Knowles et al(95) Numer Math 70. [3] Pappalardo et al(04) Appl Opt 43. [4] Russo et al (06) Appl Opt 45.

IC/PP1052/015: Double-diffusive mixed-convection in a lid-driven cavity under the counter-acting buoyancy forces.

Presenter: Dilip Maiti (Birla Institute of Technology & Science, India)

Present study deals with steady two-dimensional flow accompanied by heat and mass transport in a lid-driven square cavity filled with a mixture of a solvent vapor and non-condensable gas subjected to the vertically parallel thermal and solutal gradients. The top lid is maintained at constant speed while other three walls are kept fixed. Zero heat and mass fluxes are imposed on the vertical side walls. The governing unsteady Navier-Stokes equations combined with the heat and mass transport equations are solved numerically through a finite volume method on a staggered grid system using QUICK scheme for convective terms. The resulting equations are then solved by an implicit, time marching, pressure correction based SIMPLE algorithm. The essential details of flow, temperature and concentration fields are presented for the opposing buoyancy forces ratio $B < 0$ with special attention being given to find the values of parameters- such as Reynolds number, thermal and solutal Richardson number and the buoyancy forces ratio- for which the flow in the cavity is fully dominated by either lid-driven convection or thermal- or solutally-induced convection/conduction.

15: Modelling and Simulation, Minisymposia

IC/MP338/010: **Study groups with industry.**

Organiser: Hilary Ockendon (University of Oxford, UK)

This minisymposium will showcase the Study Groups with Industry which have been used world-wide to provide an effective mechanism to make contacts between academic mathematicians and industrial scientists. The four presentations will show how these meetings have evolved in different countries and will describe some case studies.

Industrial mathematics initiatives in the Western Pacific region. **Graeme Wake** (Massey University, New Zealand) IC/MT382/010

Since the 1980s the Australian and New Zealand Applied Mathematics fraternities have operated a Mathematics-in-Industry Study Group. After a consolidating period this annual event became a key activity of a special interest group of the Australian and New Zealand Industrial and Applied Mathematics (ANZIAM) organisation. This activity has been held in different centres in Australia and New Zealand with a view to seeding ongoing activity in each area. In 2007 it moved to the University of Wollongong in Australia and includes interactive web-based activity. This talk will review the recent activities of the ANZIAM MISGs, giving special attention to the evolving differences we have effected such as: student moderators, contract negotiations, publications, international outreach, etc. Within New Zealand efforts are being made to develop an activity modelled on the successful Smiths Institute at Oxford.

Graph colouring for office blocks. **David Allwright** (University of Oxford, UK) IC/MT384/010

Most modern office blocks have different companies working in the same building, so the use of wireless computer networks (WLAN) introduces a security problem. It is impracticable to have complete electromagnetic screening around each company's *territory*. However, BAE SYSTEMS have developed a frequency selective surface that could be used on walls and ceilings, such that transmission across *two* such interfaces would be undetectable. But companies either side of *one* wall or floor/ceiling would still need to be on *different* WLAN channels. How many channels are needed for a typical building, and how can a good assignment be found? The talk will describe how the UK Study Group addressed these questions, which are graph colouring for the adjacency graph of the 3-dimensional territories.

An interesting specific case is how many channels are needed if each territory is a cuboid (aligned with a fixed set of Cartesian axes). The talk will include Bruce Reed and Adrian Vetta's ingenious construction to answer this question, showing that for n cuboids the number of channels may need to be of order $\log\log n / \log\log\log n$, and can therefore be arbitrarily large.

Study groups in Denmark: a tale of two cities. **Poul Hjorth** (Danmarks Tekniske Universitet, Denmark) IC/MT1413/010

Since 1998 European Study Groups with Industry have been held in Denmark, and Danish companies varying from LEGO and NOVO to very small high-tech firms continue to participate. In this talk I will briefly describe the history, the organisation and the format of the Danish Study Groups, and highlight a few particularly interesting problem solutions.

Case studies from the Canadian and Chinese SGs. **Huaxiong Huang** (York University, Canada) IC/MT2251/010

In this talk we will present a few case studies on problems submitted to the Canadian and Chinese Study Groups (SGs). The Canadian SG started in 1998 (with help from OCIAM) and have been held annually in Western Canada by the Pacific Institute for the Mathematical Sciences. SG in other parts of the Canada were also held, most recently in Toronto by the Fields Institute. The Chinese SG, including the ones in Hong Kong, started in Fudan University with supports from the Chinese NSF, the Royal Society of London and OCIAM. Over the years, we have worked on problems from industry as well as from government research labs, health and medical centers and financial institutions. If time permits, some details will be given on modeling InSb crystal growth, one of the SG problems which evolved into a collaborative project and produced two PhD and one Master's dissertations.

IC/MP228/010: **On morphology of growing surface of crystals.**

Organiser: Etsuro Yokoyama (Gakushuin University, Japan)
Co-organiser: Yoshikazu Giga (University of Tokyo, Japan)

The morphological prediction of a crystal is interdisciplinary and is related to various subjects, transport and diffusion phenomena, physical chemistry of surface and interface, nucleation, chemical reactions, convection surrounding a crystal, and phase transformation, which involves a lot of mathematical problems, such as morphological instabilities. The pattern of a growing crystal depends not only on crystal structure but on conditions in the nutrient phase, e.g. temperature and concentration, which influence the growth speed of each element of the interface. In addition, the growth speed of each element depends on the local geometry of the interface, specifically on the interface curvature and the orientation of the interface relative to the crystal axes. Furthermore, the growth speed of interface is affected by impurities over the interface, and by the presence of defects of the interface. In the physics and chemistry of surface, recently, the development of numerous techniques of in situ observation is able to reveal not only step motion along the interface but diffusion of admolecules and/or impurities over the interface. The structure of growing interface has been studied using various Monte Carlo simulations and recently the model of spiral motion to occur with aid of screw dislocations is proposed using by a level set method. The formation of patterns during growth of a crystal is a difficult free boundary problem and can be solved using by numerical techniques, such as a boundary integral method, recently a phase field model and more recently a level set method. The speakers present an overview of research on morphology of growing surface of crystals both in experimental and theoretical aspects.

Evolution of polyhedral crystals. **Przemyslaw Gorka** (Politechnika Warszawska, Poland) IC/MT2714/010

We consider a system modelling evolution of a single crystal grown from vapor. We account for vapor diffusion and Gibbs-Thomson relation on the crystal surface. We also assume that the velocity of the growing crystal is determined by the normal derivatives of concentration of vapor at the surface. Mathematically speaking, this is a one-phase Stefan-type problem with the curvature and kinetic term. We show local in time existence of solutions assuming that the initial crystal is an arbitrary admissible polyhedral shape.

Crystal growth in deposited snow: experiment, physical modeling and simulation. **Frédéric Flin** (Mateo, France), Jean-Bruno Brzoska (Centre d'Etudes de la Neige, France), Yoshinori Furukawa (Hokkaido University, Japan) IC/MT2834/010

Snow, from its fall until its full melting, undergoes transformations of its microstructure with time. This process, named *metamorphism*, drastically influences its physical, thermal and mechanical properties and is of great interest in snow and ice sciences. The recent possibility of acquiring 3D images of small snow samples opens new opportunities for investigating snow in details. For this purpose, we developed specific algorithms in order to extract the relevant geometrical and physical parameters from the imaged samples (e.g. normal and curvature fields, surface area). We then used these estimators to develop 3D models that simulate the time-lapse transformations of snow directly from an experimentally observed microstructure. These models, which can be checked with experiments in cold room, offer new outlooks for the study of snow metamorphism.

Morphological stability of a growing faceted crystal. **Etsuro Yokoyama** (Gakushuin University, Japan), Yoshikazu Giga (University of Tokyo, Japan) IC/MT4183/010

We review briefly studies of morphological instability of a growing faceted crystal, in which the interplay between nonuniformity in supersaturation on a growing facet and anisotropy of surface kinetics derived from the lateral motion of steps, leads to a faceted instability, i.e., preferred growth of corners and edges of the faceted crystal. As long as the nonuniformity in supersaturation on the facet is not too large, it can be compensated for by a variation of the density of microscopic growth step along the facet. We discuss the time dependent behavior of local step density on the growing macroscopically flat facet under a given nonuniformity in supersaturation along the surface by means of the characteristics for a first order partial differential equation of growing surface and show that the asymptotic behavior of local step density can be determined by the variation of reciprocal of supersaturation under the conditions of stability.

Multi-phase systems with anisotropic surface energies and volume constraints. **Björn Stinner** (University of Sussex, UK) IC/MT4321/010

The dynamics of phase boundaries in multi-phase systems has been studied with a focus on interfacial energy contributions. The aim has been a diffuse interface description based on the phase field methodology which, in the sharp interface limit, is related to a classical description with moving hypersurfaces modelling the phase boundaries. A nontrivial task in the case of multiple phases is to let surface quantities as (possibly anisotropic) surface energies and mobility coefficients enter the equations of the diffuse interface model in the right way. Volume constraints for (some of) the phases lead to nonlocal partial differential equations. Depending on the multi-well potential used for the phase field equations several numerical methods will be presented taking that constraints into account.

IC/MP257/015: Modeling and simulation for nano-scale materials.

Organiser: Luis Bonilla (Universidad Carlos III de Madrid, Spain)
Co-organiser: Russel Caflisch (University of California, Los Angeles, USA)

The nanoscale physics and structure of materials are of vital importance for modern science and technology. Examples include microelectronic devices and possible successors to CMOS technology, strength and plasticity of materials, and high-speed sensors. Modeling and simulation for nanoscale materials faces considerable challenges because of their complexity, as well as their dependence on multiple length and time scales (ranging from Angstroms and femtoseconds to centimeters and seconds) and multiple physics descriptions. This minisymposium will focus on new analytic, modeling and simulation methods for nanoscale materials, in particular for defects in these materials. Defects (for example cracks, dislocations, stacking faults and substitutional defects) can have significant, even determining, effects on material strength, reliability of device properties and self-assembly of structures. The presentations in the minisymposium are as follows.

The first talk describes a novel algorithm for kinetic Monte Carlo simulations which is based on exact Green's functions of the theory of first-passage processes and is applicable to a wide range of physical situations where multiple Brownian particles of finite dimensions diffuse, collide and react with each other. Applications include Oswald ripening, semiconductor processing, defect microstructure evolution in fusion and fission reactor materials, and diffusion-controlled reactions in confined geometries.

The second talk deals with discrete models of defects in crystal lattices, which are the basis of macroscopic properties such as the strength of materials and control their mechanical, optical and electronic properties. Discrete models will be used to study the interaction and motion of dislocations, and to define and analyze dislocation densities.

The third presentation will discuss the role of dislocations and alloying in self-assembly and directed self-assembly for quantum dots, using a level-set method to simulate epitaxial growth and an algebraic multigrid method for the simulation of atomistic strain. These methods are designed to include both continuum and atomistic length scales.

The fourth talk will concern non-separability of length scales in solid mechanics, due to severe nonlinearity, and its role on multi-stability of a mechanical system at a micro-level.

First passage Monte-Carlo: diffusion without all the hops. **Vasily Bulatov** (Lawrence Livermore National Laboratory, USA), Tomas Oppelstrup (NADA, KTH-Royal Institute of Technology, Sweden), Aleksandar Donev (Lawrence Livermore National Laboratory, USA), Babak Sadigh (Lawrence Livermore National Laboratory, USA), Malvin Kalos (Lawrence Livermore National Laboratory, USA), George Gilmer (Lawrence Livermore National Laboratory, USA) IC/MT1477/015

We present a novel Monte Carlo algorithm for N diffusing particles of finite sizes that react on collisions. Using the solutions of the theory of first passage processes and time dependent Green's functions, we break the difficult N-body problem into independent single- and two-body propagations circumventing numerous diffusion hops used in standard Monte Carlo. The new algorithm is exact, extremely efficient and applicable to many important physical situations in arbitrary integer dimensions.

Rate-independent plasticity and criticality. **Lev Truskinovsky** (École Polytechnique, France) IC/MT1733/015

We show that the classical singular dissipative potential of the phenomenological rate independent plasticity can be obtained by homogenization of a micro-model with quadratic dissipation. The essential ingredient making this reduction possible is a rugged energy landscape at the micro-scale, generating under external loading a cascade of subcritical bifurcations. Such landscape may appear as a result of a sufficiently strong pinning or jamming of defects, leading to elastic micro-metastability. The homogenized system behaves as marginally stable or critical. Already in two dimensions the criticality manifests itself through power law acoustic emission.

Growth and pattern formation for thin films. **Russel Caflisch** (University of California, Los Angeles, USA) IC/MT2075/015

Growth of an epitaxial thin film involves physics on both atomistic and continuum length scales. For example, diffusion of adatoms can be coarse-grained, but nucleation of new islands and breakup for existing islands are best described atomistically. The lattice properties of the film are determined by those of the underlying substrate. In heteroepitaxial growth, e.g., Germanium on Silicon, mismatch between the lattice spacing of the Silicon substrate and the Germanium film will introduce a strain into the film, which can significantly influence the material structure, leading for example to the formation of quantum dots. Technological applications of quantum dot arrays require a degree of geometric uniformity that has been difficult to achieve. One approach to overcoming this difficulty is to prepattern the system, for example with buried dislocation lines. This talk will describe mathematical modelling, simulation methods and computational results for epitaxial growth, strain in thin films and pattern formation. The growth simulations use an island dynamics model with a level set simulation method. Strain computations can be computationally intensive, so that effective simulation of atomistic strain effects relies on an accelerated method that incorporates algebraic multigrid and an artificial boundary condition. Simulations that combine growth and strain will be presented showing spontaneous and directed self-assembly of patterns (quantum dots and wires) on thin films.

Dynamics of defects in crystal lattices and bifurcation theory. **Luis Bonilla** (Universidad Carlos III de Madrid, Spain), Ana Carpio (Universidad Complutense de Madrid, Spain) IC/MT2363/015

Crystal defects such as dislocations are the basis of macroscopic properties such as the strength of materials and control their mechanical, optical and electronic properties. Advances in electronic microscopy have allowed imaging of atoms and therefore to visualize the core of dislocations, cracks, and so on. In continuum mechanics, dislocations are treated as source terms proportional to delta functions supported on the dislocation line. Cores and crystal structure are not properly considered and it is hard to describe the motion of crystal defects. Unlike defects in fluids (such as vortices), dislocations move only within glide planes, not in arbitrary directions, and they move only when the applied stress surpasses the Peierls stress, which is not infinitesimal.

We have proposed a discrete model describing defects in crystal lattices with cubic symmetry and having the standard linear anisotropic elasticity (Navier equations) as its continuum limit. Moving dislocations are traveling waves which become stationary solutions if the applied stress falls below the Peierls value. The corresponding transition is a global bifurcation of the model equations whose type depends on whether the chosen dynamics includes dissipation. In addition, homogeneous nucleation of dislocations occurs when a sufficient shear stress $F > F_c$ is applied to a dislocation-free crystal. Then the strained dislocation-free state becomes unstable via a subcritical pitchfork bifurcation at $F = F_c$. The bifurcation diagram is studied by numerical continuation and a mechanism to select simultaneously stable configurations containing different number of edge dislocations is analyzed.

IC/MP641/015: Mathematical, computational and statistical modelling in metrology.

Organiser: Maurice Cox (National Physical Laboratory, UK)
Co-organiser: Alistair Forbes (National Physical Laboratory, UK)
Co-organiser: Markus Bär (PTB-Berlin, Germany)

Metrology, the science of measurement, is fundamental to a vast range of activity worldwide, providing critical support for manufacturing, quality of life, health, environment and climate change as well as all major scientific disciplines. The annual expenditure on measurement within the European Union alone is estimated to be over 80 billion euros (100 billion USD). Metrology has drawn heavily from many mathematical disciplines, including applied mathematics, numerical analysis, optimisation and data approximation. In recent years, the importance of developing valid statistical models associated with measurement systems has been recognised in order that scientific inferences (e.g., uncertainty statements, go/no-go decisions) made on the basis of measurement data are reliable. Much of quantitative analysis in metrology now occupies an interesting and challenging intersection of mathematics and probability theory. In parallel, advances in algorithms and computational methods open up the possibility that the outcome of measurements can be obtained from simulation of suitable mathematical models (*virtual experiments*). If metrology is currently seen as mainly an experimental science, the role of computation is increasing. This mini-symposium will report on recent advances in the application of mathematical, computational and statistical modelling to metrology, especially in the areas of modelling measurement systems, parameter estimation, the propagation of distributions and uncertainty evaluation, and the design and analysis of interlaboratory comparisons.

Mathematical modelling and measurand identification required for defining mises en pratique *of the Kelvin.* **Franco Pavese** (Consiglio Nazionale delle Ricerche, Italy), Daniela Ichim (Istituto Nazionale di Statistica, Italy) IC/MT4091/015

For some physical quantities, the method of defining mises en pratique of the unit for practical standards is used, allowing one or more defined implementations. This was in 2005 the case of temperature by transforming ITS90 and PLTS2000 into two mises en pratique, with possible further mises en pratique in future. Temperature, as an intensive quantity, requires the definition of a scale as the actual measurement standard. One possible future direction for mises en pratique is to furtherance the realisations of the thermodynamic scale that so far only represented the physical bases of the definition of the empirical scales. A second one is arising from the fact that the addition of further mises en pratique only requires all being compatible with each other, to avoid ambiguities in the definition of the temperature values. Other scales that presently are approximations for the ITS90 could become mises en pratique, also for lower accuracy levels. In addition, the use of mises en pratique can alleviate presently conflicting issues about measurand definition in comparisons. A big variety of modelling requirements corresponds to the variety of definitions: in fact they range from thermodynamic ones, requiring a correct physical modelling, to semiempirical, to empirical ones. Since temperature can be measured only by measuring another physical quantity, e.g., electrical resistance, pressure, a change in length, etc., the measurand related to each of the above definition must be correctly and clearly identified, which can be less obvious than it might look. The presentation will first introduce the general thermometric problem, limited to making the subsequent illustration of the problems concerning measurand identification and modelling issues understandable. Then it will summarise the correct procedures to correctly and clearly identify the measurand of each given definition, whith examples of possible ambiguities. Finally it will illustrate the characteristics of the main families of models suitable for use in temperature scales, used or candidates for use as mises en pratique of the kelvin, from the viewpoint of the metrologist, concerning either the mathematical requirements and the requirements of the statistical treatment of the experimental temperature data.

Challenges for mathematical and statistical modelling for metrology. **Maurice Cox** (National Physical Laboratory, UK), Alistair Forbes (National Physical Laboratory, UK), Peter Harris (National Physical Laboratory, UK) IC/MT4149/015

A glance through recent volumes of journals such as *Metrologia*, *Measurement*, and *Measurement Science and Technology* indicates the considerable extent to which mathematical and statistical modelling are used in metrology. Seven volumes of *Advanced Mathematical and Computational Tools for Metrology*, resulting from conferences in the area, reinforces this view. Publication of a special issue of *Metrologia*, with a number of downloads in the month following publication double that for a typical issue, provides further evidence of the relevance of statistical methods for metrology.

This paper looks at three aspects of the mathematical and statistical treatment of measurement problems and associated journal articles.

One, who writes these articles? Who uses them and to what extent? How large is the take-up gap between the relatively academic presentation of the writer and the sometimes limited mathematical and statistical knowledge of the practising metrologist as reader? Are there better ways of conveying information?

Two, do the published articles address actual problems of metrological concern? The answer is “yes” in some but not all respects. Do the solutions proposed account for the measurement information available, or turn a blind eye to part of it in order to derive a simpler solution?

Three, to what extent do paper writers and practising metrologists form distinct camps? Co-working is improving, but not at a rapid rate. Development of a mathematical or statistical model requires the involvement of both parties to maximize its value. A key area is uncertainty evaluation in the context of a model of measurement, where quantifying and coping with uncertainty structures benefits from joint consideration by all concerned.

This paper discusses the challenges implied by these questions.

Atomistic modelling in metrology: algorithms and current challenges. **Vlad Sokhan** (National Physical Laboratory, UK) IC/MT4175/015

Mathematical modelling plays an increasingly important role in measurement science where many problems of fundamental and practical importance require solutions at meso and nano scales. In quantum and materials metrology atomistic simulation has developed to a level where it is competing in accuracy with laboratory measurements.

In this talk an overview of recent algorithmic development and applications of atomistic simulation to problems of metrology will be given.

Uncertainty evaluation for parametric and semi-parametric modelling. **Clemens Elster** (PTB-Berlin, Germany) IC/MT4277/015

Uncertainty evaluation for parametric modelling is considered in the context of regression analysis. Application of maximum likelihood as well as Bayesian statistics are discussed for parameter estimation in the context of particular metrology-relevant aspects such as the presence of non-random (systematic) measurement errors.

The extension of parametric to semi-parametric modelling is considered for the task of spectral analysis. The particular semi-parametric model to be treated requires the estimation of a smooth baseline signal in addition to the adjustment of a parametric model for the spectrum. A regularization approach is proposed leading to a spline solution for the baseline. The regularization approach is regarded from a Bayesian point of view which is then used for uncertainty evaluation. The particular semi-parametric modelling approach is finally illustrated by means of an example from NMR spectroscopy.

IC/MP641/015: Mathematical, computational and statistical modelling in metrology. #2

Organiser: Maurice Cox (National Physical Laboratory, UK)
Co-organiser: Alistair Forbes (National Physical Laboratory, UK)
Co-organiser: Markus Bär (PTB-Berlin, Germany)

(For abstract, see session #1 above.)

Partial differential equations and inverse problems in metrology (overview talk). **Markus Bär** (PTB-Berlin, Germany) IC/MT4278/015

Many measurement systems are adequately modelled by partial differential equations (PDEs). This talk describes various applications of PDEs models in metrology. In the first part, general aspects of PDEs in metrology and the use of well-established models like the heat equation or Maxwell’s equation for current metrological applications is reviewed. The emphasis is on the realization of "virtual experiments" and, in particular, on the demand of solving inverse problems. This

is needed in many modern metrological applications in order to determine material or geometry parameters of a given unknown probe. In more detail we will report on recent progress in solving the inverse problem for scatterometry of visible light and extreme UV radiation at masks employed in chip production. Finally, we will address the problem of a proper metrological treatment of a much more complex system of partial differential equations, namely the quantitative modelling of electric and magnetic phenomena in human and animal hearts. First steps towards a quantitative heart modelling based on measurements of physiological and anatomical parameters are presented for the examples of a rabbit heart and a human heart. The simulation results are compared to measurements of electric potentials on the surface of isolated hearts as well as to electro- and magnetocardiographic recordings.

Joint work with: S. Bauer, H. Gross, R. Model (PTB Berlin, Germany) and A. Rathsfeld (Weierstrass-Institute of Applied Analysis and Stochastics, Berlin, Germany)

Propagation of uncertainties in measurements using fiducial inference. **Chih-Ming Wang** (National Institute of Standards & Technology, USA), Hari Iyer (National Institute of Standards & Technology, USA) IC/MT4315/015

We present an alternative approach to the ISO *Guide* for evaluating uncertainty in measurements. The approach, based on FisherŠs fiducial arguments, can easily and naturally incorporate both type-A and type-B information into the model assumptions, and calculate the uncertainty for a measurand of interest. The approach can be applied to measurement models having vector-valued input quantities and measurand, and generally makes use of Monte Carlo simulation to evaluate measurement uncertainty. Examples are used to illustrate the procedure.

A novel approach using parallel Kalman filters in time and frequency estimation. **Ragne Emardson** (SP Technical Research Institute of Sweden) IC/MT4564/015

Accurate knowledge of time and frequency plays a fundamental role in many applications in our information based knowledge society. UTC, which is the basis of world time distribution, is a combination of the atomic time scale TAI and earth rotation information. TAI is calculated by the International Bureau of Weights and Measures (BIPM) in Paris as a weighted average of more than 200 atomic clocks. As the definition of swedish national time is based on UTC, good estimates of a clock's deviation from UTC is crucial for high-performance time keeping. For many applications, real time estimates of the clock's time and frequency error are required. We have developed a novel approach for estimating time and frequency errors based on a assembly of clocks of varying quality. This approach is based on using parallel Kalman filters in order to utilize all available measurements in the estimation. As these measurements are available with different delays, the Kalman filter produce estimates of different quality. One filter may produce real-time estimates while another filter waits for more measurements. When new information becomes available, the parallel Kalman filters exchange information in order to keep the state matrices updated with the most recent information. In Kalman filtering accurate modelling of the measurement system is fundamental. All the contributing clocks, as well as the time transfer methods, are modelled as stochastic processes. By using this methology, we can at every epoch obtain "optimal" estimates of time and frequency errors of a specific clock. By correctly modelling the contributing clocks and time transfer links, we may also estimate the uncertainty of each time and frequency estimate.

IC/MP706/015: Wave structures and complex dynamics in models of highway traffic.

Organiser: Richard Wilson (University of Bristol, UK)

The modelling of highway traffic is an area of huge economic importance: in the UK alone, it is estimated that traffic jams cost the economy more than 20bn GBP annually. Furthermore, there is a general trend in using information and communication technology to try to influence driver behaviour and control congestion. However, despite over 50 years of research, there is still a need to improve the basic understanding of the dynamics of highway traffic. A lot of interesting questions remain both in terms of modelling and in terms of mathematical analysis.

In the literature there are very many models of highway traffic, and these may be classed as either macroscopic (averaged and fluid-like, usually PDEs) or microscopic (modelling vehicles at the individual level). Moreoever, there are subdivisions of these classes and overlaps between them. For example, the microscopic class breaks down into car-following models (which consider vehicles to be discrete entities moving in continuous time and space) and cellular automata models (where vehicles, time and space are discrete and where dynamics are driven by stochasticity). There are however connections across the scales between the different model types; for example, the emergent macroscopic dynamics of car-following models may be described by PDEs.

This minisymposium will provide a melting pot where practitioners of the different modelling approaches are brought together. We will explore the underlying mathematical mechanisms for the complex dynamics that models exhibit, and we will seek connections across the scales between different model types. Comparisons with empirical traffic data will also be sought. Hence we anticipate that this minisymposium will help lay the foundation stone of a new multiscale framework for understanding traffic flow.

Spatio-temporal pattern in highway traffic: empirical data and modelling approaches. **Richard Wilson** (University of Bristol, UK) IC/MT3955/015

In this talk I will describe the key spatio-temporal features of empirical highway-traffic data and I will summarise their 50 year old modelling history. I will then focus on the nonlinear behaviour of microscopic car-following models in particular, and I will show how dynamical systems techniques may be used to understand the fundamental mechanisms behind traffic jam generation. Finally, I will illustrate connections to macroscopic PDE theory and outline possible future directions.

Rigorous techniques for analyzing CA traffic models. **Lawrence Gray** (University of Minnesota, USA) IC/MT3357/015

Cellular automata (CA) were first used to model traffic by Nagel and Schreckenberg. These models are discrete, both in space and in time, and yet they exhibit many of the interesting complex phenomena that are characteristic of actual traffic. Their discrete nature makes them easy to describe and easy to simulate.

During the past few years, techniques have been developed for rigorous mathematical analysis of CA traffic models, primarily for a variation on the Nagel-Schreckenberg model introduced by Gray and Griffeath. This analysis brings a number of other particle models into play, including the "branching annihilating random walk" and the "chipping model". Comparisons between models are facilitated by a mathematical technique known as "coupling". Standard coupling methods have not been applica-

ble to most CA traffic models, but recent ideas have changed this.
These new ideas will be described, and it will be seen that the resulting mathematics provides some insights into the phenomena that make traffic so interesting.

Some microscopic–macroscopic problems arising in the mathematical study of second order models of traffic flow. **Michel Rascle** (Université de Nice, France), Salissou Moutari (Université de Nice Sophia Antipolis, France) IC/MT3895/015

I will first describe various aspects of mathematical and modeling problems arising (in particular) in the description of traffic flow by the class of fluid "second order" models, introduced several years ago in Aw-Rascle, SIAP, 2000 ("Resurrection"), in connection with the celebrated ("Requiem ...") paper of Daganzo in 1995.
This class of models is the natural extension of "first order models", i.e. of scalar conservation laws. Moreover, they are also the (rigorous) limit of discrete Follow-the-Leader Models in a hyperbolic scaling : $(x,t) \to (\varepsilon x, \varepsilon t)$, as shown with Aw, Klar and Materne, SIAP 2002.
In recent years, there has been a large amount of work devoted to apply these various types of models to realistic situations, such as junctions, networks, complex flows etc., and/or to combine them via hybrid schemes. Depending on the time, I will describe some of these aspects.

Travelling waves on lattices defined by car-following models. **Antony Humphries** (McGill University, Canada) IC/MT4999/015

We consider the dynamics of microscopic car-following models on an infinite highway. Such models take the form of a lattice differential equation system, whose travelling wave solutions are defined by a delay differential equation boundary value problem. When reaction times are included, advanced-retarded FDE problems arise. We will use manifold dimension counting arguments to analyse the genericity of such solutions, and numerical continuation techniques determine domains of existence and solution forms, and identify connections with macroscopic PDE traffic theory.

IC/MP706/015: Wave structures and complex dynamics in models of highway traffic. #2

Organiser: Richard Wilson (University of Bristol, UK)

(For abstract, see session #1 above.)

Three characteristic times: how the reaction time, the update time, and the adaptation time influence stability of traffic flow. **Martin Treiber** (TU Dresden, Germany) IC/MT3897/015

In the context of microscopic traffic models, there are three characteristic time constants that influence the dynamics and stability of traffic flow: The reaction time of the drivers, the velocity adaptation time needed to accelerate to a new desired velocity, and the numerical update time. In spite of their conceptual differences, these times are often confused. Particularly, the update time of iterated maps (such as the Newell model) or the adaptation time of time-continuous models (such as the optimal velocity model) are often treated as a 'reaction time'. In this contribution, we numerically investigate how these times influence the local and string stability of a platoon of vehicles. In particular, we found that the numerical update time is dynamically equivalent to half the reaction time. Furthermore, with respect to stability, there is an 'optimal' adaptation time as a function of the reaction time.

Multi-lane models of traffic flow across the scales. **Jon Ward** (University of Bristol, UK) IC/MT3609/015

Motorway traffic is a discrete dynamical system of interacting particles. However, many mathematical approaches model it as a continuum with fluid-like properties. In this talk we will investigate how multi-lane microscopic models of traffic flow can be used to infer desirable properties for equivalent macroscopic models. We will also analyse how spatio-temporal phenomena express themselves in models of different scales.

A hybrid Lagrangian scheme for vehicular traffic flow. **Salissou Moutari** (Université de Nice Sophia Antipolis, France) IC/MT5057/015

In this talk, we will present a simple fully discrete hybrid model for vehicular traffic flow, based on a Lagrangian discretization of the Aw–Rascle model[1]. The main idea is to combine the microscopic description of the traffic (around an obstacle such as traffic light, toll station, intersections, etc.) with a macroscopic description (away from the obstacles). Due to the Lagrangian modelling, we have no lost or gain of mass at the interfaces. We will briefly describe how to establish the BV estimates for the whole hybrid model. Finally we will present some few numerical simulations of this hybrid scheme in the case of traffic light, especially with different CFL conditions in the microscopic and macroscopic regimes.

[1] Aw, A. and Rascle, M.; SIAM J. Appl. Math., 60 (2000).

Calibration of microscopic traffic-flow models: what can be learned for the wave-structure formation on highways?. **Peter Wagner** (German Aerospace Center, Germany) IC/MT3400/015

By using the trajectory data provided by the NGSIM project, the parameters of microscopic models could be calibrated to the data at hand. Several possibilities to do this are discussed and tested, which leads to a whole distribution of the parameters of the model in use. After doing so, it could be discussed which kind of traffic pattern could be reproduced with which kind of microscopic traffic flow model, and, more interestingly, what can not be reproduced. This should shed light on the ongoing discussion about the traffic flow patterns called synchronized traffic flow, to help understanding its nature.

IC/MP711/010: The mathematics of food: modelling and computation.

Organiser: Arthur Parrott (University of Greenwich, UK)
Co-organiser: Andrew Lacey (Heriot-Watt University, UK)

There is a growing interest in applying mathematics to the solution of problems arising out of food engineering, an area traditionally dominated by experimental approaches. This minisymposium focuses on problems where the complexity either of the food material or of the process or both leads to interesting and challenging problems either in mathematical or computational modelling. In many cases there are specific food-related features that dictate a novel approach to the solution and the use of conventional Heat Transfer and CFD packages is not possible. Examples of this type of problem include texture development governed by internal moving boundaries in foam-like dough during baking, domestic microwave thawing requiring a coupled computational approach with both computation of heat transfer and the numerical solution of MaxwellŠs equations in moving domains, scraped surface heat exchangers where heat transfer and flow occur on a very wide range of length scales and the frying of porous materials where detailed modelling results in non-standard moving boundary problems.

Crust formation in bread baking. **Andrew Lacey** (Heriot-Watt University, UK) IC/MT3466/0

A model for the formation of a crust during bread baking is presented. The crust is the outermost part of the loaf where the final bread density is significantly higher than in the interior of the loaf, called the crumb. Our model is based on a collapse mechanism, whereby raised pressures in the interior part of the loaf, due to thermal expansion and water evaporation, squash bubbles in the outer part of a bread loaf at the same time as the bread sets and fractures. The latter process allows vapour to escape from bubbles which can then shrink.

Mathematical models for frying processes. **Mario Primicerio** (Università degli Studi di Firenze, Italy) IC/MT3568/0

We present mathematical models for the process of frying a rather thick sample of an non-deformable porous material saturated with water (e.g. a potato slice). The models are based on thermodynamical arguments and result in a class of initial-boundary value problems for a system of equations satisfied by the temperature, pressure and vapour content; in the case of one-dimensional geometry, the domain in the x-t plane is decomposed in subregions where the porous medium may be totally saturated, partially saturated, or completely dry. Correspondingly, the free boundary conditions are discussed. We provide a preliminary analysis and present some results of numerical simulations

Microwave modelling and validation in food-thawing applications. **Arthur Parrott** (University of Greenwich, UK), Tim Tilford (University of Greenwich, UK) IC/MT4229/0

Thawing of a frozen food product in a domestic microwave oven is simulated numerically using a coupled solver approach. The approach utilises a dedicated electromagnetic FDTD solver which is closely coupled to an unstructured FVM multi-physics package. Two overlapping numerical domains are defined; the food material and container were meshed for heat transfer and phase change solution, whilst the microwave oven cavity and waveguide are meshed for the microwave irradiation. The two solution domains are linked using a cross-mapping routine. This approach allows the rotation of the food load to be captured. Power densities obtained on the structured FDTD mesh are interpolated onto the unstructured FVM mesh for each time-step/turntable position. The FVM solver utilises the power density data to advance the temperature and phase distribution solution. The temperature-dependant dielectric and thermo-physical properties of the food load are updated prior to revising the electromagnetic solution. Changes in thermal/electric properties associated with the phase transition were fully accounted for as well as heat losses from product to cavity. Two scenarios were investigated: a centric and eccentric placement on the turntable. Developing temperature fields predicted by the numerical solution are compared against experimentally obtained data. Presented results indicate the feasibility of fully coupled simulations of the microwave heating of a frozen product. The agreement between numerical and experimental solutions is good whilst the food is frozen, but deteriorates after thawing. The variation in heating pattern due to eccentric placement is shown.

IC/MP669/151: Dynamics of cutting processes.

Organiser: David Barton (University of Bristol, UK)

Machining operations, such as high-speed milling or drilling, are among the most widely used of all manufacturing processes. Cost efficiency and accuracy are important, however high-performance machining is prone to self-excited chattering behaviour which leads to increased tool wear, inferior surface quality and poor dimensional accuracy. Furthermore, at the most efficient parameter settings, chattering motions can occur spontaneously, hence automated processes are often planned conservatively.

This mini-symposium is focused on understanding the dynamics (both linear and nonlinear) of different cutting operations and using this knowledge to improve the efficiency while maintaining accuracy and surface quality. It will start with an overview of the subject area, which will then be followed by a series of talks focusing on modelling, analysis, and experimental investigation of different cutting operations. Particular emphasis is placed on the study of the fly-over effect during chatter and associated non-smooth behaviour including the bifurcations that cause its onset.

The nonlinear dynamics of cutting processes. **Gabor Stepan** (Budapest University of Technology and Economics, Hungary) IC/MT2574/151

Time delay tends to destabilize any dynamical system. This is not true, however, in case of delayed oscillators, which serve as mechanical models for lots of surprising physical phenomena. Parametric excitation of oscillatory systems also leads to stability properties sometimes opposite to our physical sense. The combination of the two effects is a challenging task to predict nonlinear dynamic behaviour in these systems. Referring to the infinite dimensional nature of the dynamics of cutting subjected to regenerative effect, its nonlinear vibrations are often compared to the problem of turbulence in fluid mechanics.

In case of turning, the linear stability analysis of stationary cutting provides complicated, sometimes fractal-like stability charts in the space of the technological parameters (cutting speed, depth of cut and feed rate). Some experiments predicted the existence of unstable periodic motions around the stable stationary cutting already in the early 80Šs, but the corresponding subcritical co-dimension 1 and 2 Hopf bifurcations in turning processes have been shown analytically only recently. The description of the global dynamics of the cutting process ŚoutsideŠ the unstable limit cycles or unstable tori requires the analysis of the so-called self-interrupted cutting, when the time-intervals of the no-contacts between the tool and the workpiece are regulated by the system itself.

Milling is a kind of cutting where loss of contact between the teeth of the tool and the work-piece occurs typically in a periodic way. This leads to non-autonomous governing equations

similar to the damped, delayed Mathieu equation. The parametric excitation in the delay-differential equation yields secondary Hopf (or Neimark-Sacker) bifurcations, and also period doubling (or flip) bifurcations, when the cutting speed is high enough. The global nonlinear dynamics of turning and high-speed milling are compared as self-interrupted and parametrically interrupted cutting processes.

Analytical modeling of chatter stability using multi-dimensional approach. **Erhan Budak** (Sabanci University, Turkey) IC/MT2472/151

Chatter is one of the main problems in machining resulting in poor surface finish and low productivity. Stability models can be used to determine stable cutting conditions with higher productivity. Although majority of the machining systems involve muti dimensional dynamics, most of the stability models consider a single dimension in the formulation. This seminar willl give a brief overview of the multi dimensional models that we have developed for turning, boring and milling processes. The turning stability model considers the tool and part dynamics in two directions as well as insert nose radius. The model for milling involves stability analysis of time varying multi dimensional system which is solved analytically. Experimental results and industrial will be presented for different processes. Finally, methods for machine tool dynamics measurement and modeling will be discussed.

Surface errors for helical mills. **Dániel Bachrathy** (Budapest University of Technology and Economics, Hungary), Gabor Stepan (Budapest University of Technology and Economics, Hungary) IC/MT1083/151

Stability and surface location error are investigated numerically for milling operations with helical tool. A detailed mechanical model is derived that includes both surface regeneration and the helical teeth of the tool. The governing delay-differential equation is given in closed form and is analyzed by the semi-discretization method. The surface location error is predicted based on the forced motion of the tool for different axial depths of cut. The relationship of the spectrum of the cutting force and the surface properties is described. It is shown that the surface location error is varying periodically along the axial direction due to the helical teeth.

Phase-locked and quasi-periodic vibrations in a high-speed milling process. **Robert Szalai** (University of Bristol, UK) IC/MT2276/151

Milling processes are common in industry as they can achieve fast and high precision manufacturing. They are frequently used in the automotive and aerospace industry, where parts with difficult geometry are produced. Despite the efficiency these processes are not always reliable since they tend to exhibit unwanted vibrations due to disturbances. This stability loss is usually attributed to either the period doubling or the classical Hopf instabilities, which are subcritical. In this talk we focus on quasi-periodic and phase-locked periodic motions that arise at secondary Hopf bifurcations. Models of machining processes, due to the surface regeneration, are formulated as delay-differential equations. We introduce a method to compute quasi-periodic solutions as invariant tori in these models. These solutions are defined by a first order delayed partial differential equation, which is solved by a spectral collocation method. Using pseudo arclength continuation which keeps the rotation number fixed and follows the two technological parameters we determine phase locked regions in the stability chart.

IC/MP669/151: Dynamics of cutting processes. #2

Organiser: David Barton (University of Bristol, UK)

(For abstract, see session #1 above.)

Bifurcation in material flow during high-speed machining. **Timothy Burns** (National Institute of Standards and Technology, USA) IC/MT2793/151

A high-speed machining operation provides an interesting setting for the study of plastic flow under extreme conditions. In the thin primary shear region where cutting takes place, it is not uncommon, in alloys of interest in manufacturing, to have strains on the order of 1-10, strain rates on the order of 10^4 to 10^5 s^{-1}, and heating so rapid that the local workpiece temperature increases from ambient to a significant fraction of the melting temperature on the order of a tenth of a second or less. The thin metal strip, called a chip, which is removed during a machining operation, provides a record, i.e., a time series history, of the deformation that takes place during the cutting process. Examination under a microscope shows that chip structures can vary, depending upon the cutting conditions, from a fairly smooth case with little structure, called a continuous chip, to an extreme case with a highly periodic structure that results from repeated adiabatic shear band formation, called a shear-localized chip. In a series of papers with M.A. Davies over the past decade, ideas from nonlinear dynamics theory have been applied to model NIST experimental results on the complex evolution of the chip structure from continuous to shear-localized with increasing cutting speed. Recent improvements in high-speed micro-videography in infrared and visible wavelengths have enabled experimental measurements to be obtained at NIST of chip formation as it occurs in the plane strain setting of orthogonal cutting. New experimental results and attempts to model them from the point of view of nonlinear dynamics will be discussed.

Large-amplitude nonlinear vibration in regenerative turning model. **Zoltán Dombóvári** (Budapest University of Technology and Economics, Hungary), Richard Wilson (University of Bristol, UK), Gabor Stepan (Budapest University of Technology and Economics, Hungary) IC/MT1086/151

Self-excited nonlinear vibrations occurring in machining processes are investigated. Our treatment applies analytical and numerical techniques to a one degree of freedom but strongly nonlinear mechanical model of the turning process. This enables us to describe and analyse the highly nonlinear dynamics of the appearing periodic and more complicated motions. Using normal form calculations for the delay-differential equation model, we prove that the low-amplitude vibrations are unstable all along the stability boundaries due to the subcriticality of Hopf bifurcations. This means that self-excited vibrations of the machine tool may occur below the stability boundaries predicted by the linear theory. Zones of bi-stability are presented in the traditional stability lobe diagram.

Numerical tools for understanding chattering behaviour in non-smooth DDE models. **David Barton** (University of Bristol, UK) IC/MT2462/151

Cutting processes, such as turning or high-speed milling, often exhibit non-smooth behaviour in the form of chattering motion. Chattering is a self-excited instability where the machine tool repeatedly loses and re-establishes contact with the workpiece, causing degradation of the workpiece. Models of turning or milling that include the effects of chatter are frequently derived as systems of non-smooth delay differential equations (DDEs). However, numerical methods for the analysis of these systems are currently very limited. Often, only numerical simulation is possible.

In this talk we will demonstrate a new method for the numerical continuation of non-smooth solutions of DDEs, where the solutions are found via the solution of a multi-point boundary value problem. Numerical continuation allows a picture of the global dynamics to be built up, including any bifurcations and stability changes, and so increase our understanding of the model behaviour under parameter variations. This new method will be illustrated with the example of a regenerative turning model where chaotic chattering motion is caused by a non-smooth grazing bifurcation.

Harvesting nonlinear dynamic interactions for vibration enhanced drilling. **Marian Wiercigroch** (University of Aberdeen, UK) IC/MT3546/151

We will show how the nonlinear dynamic interactions can be used to enhance the material removal rate (MRR) and the accuracy of drilling brittle materials. First ultrasonic percussive drilling with diamond-coated tools [1] will be discussed where extensive theoretical and experimental studies conducted under laboratory conditions on rocks such as sandstone, limestone, granite and basalt, in order to investigate the applicability of this technique to downhole drilling. The experimental investigations showed that an introduction of high-frequency axial oscillations significantly improves MRR, which is strongly dependent on the static load has at least one maximum. These findings were confirmed theoretically using a simple drifting oscillator [2].

1. Wiercigroch, M., Wojewoda, J. and Krivtsov, A.M. 2005 Journal of Sound and Vibration 280(3-5), 739-757. Dynamics of ultrasonic percussive drilling of hard rocks.

2. Pavlovskaia, E.E., Wiercigroch, M. and Grebogi, C. 2004 Physical Review E 70, 036201. Two dimensional map for impact oscillator with drift.

IC/MP623/015: Mathematics for steel manufacturing.

Organiser: Dietmar Hömberg (Weierstraß-Institut Berlin, Germany)
Co-organiser: Michael Wolff (Universität Bremen, Germany)

Steel is still the most important construction material in industrial societies. One reason is that one can change its physical properties by thermal treatment, due to solid solid phase transitions. This is utilized for industrial applications in the heat treatment of steel.

The goal of the minisymposium is to show how mathematics can contribute to a deeper understanding of the occuring phase transitions and how modern methods of optimal control of pdes can be utilized for a descent description of heat treatments.

The first part is focused on the continuum mechanical modelling of phase transitions in steel, its mathematical analysis and on the optimal control of thermomechanical phase transition models.

The second part is concerned with the mathematical analysis, efficient numerical simulation and optimal control of three different surface heat treatment processes: laser, induction and case hardening.

The third part deals with the welding of steel. Here the focus is on optimization of laser welding and the analysis of a joule heating problem related to resistance welding.

Analysis of a thermomechanical phase transition model. **Krzysztof Chełmiński** (Warsaw University of Technology, Poland) IC/MT2550/152

Subject of the talk is a macroscopic thermomechanical model of phase transitions in steel. Effects like transformation strain and transformation plasticity induced by the phase transitions are considered and used to formulate a consistent thermomechanical model.

The resulting system of state equations consists of a quasistatic momentum balance coupled with a nonlinear stress-strain relation, a nonlinear energy balance equation and a system of ordinary differential equations for the phase volume fractions.

We prove the existence of a unique weak solution using fixed-point arguments. A key issue is a regularity analysis for the mechanical subsystem to obtain continuity of the stress tensor. Finally, we depict some results of numerical simulations.

Analysis of a Joule-heating model related to resistance welding. **Francisco Ortegón Gallego** (Universidad de Cádiz, Spain), María Teresa González Montesinos (Universidad de Cádiz, Spain) IC/MT1473/152

The heat produced by an electrical current passing through a conductor device is governed by the so-called thermistor problem. This problem consists in a coupled system of nonlinear parabolic–elliptic equations, whose unknowns are the temperature inside the conductor, u, and the electrical potential, φ, namely

$$\begin{aligned} \frac{\partial u}{\partial t} - \nabla\cdot(a(u)\nabla u) &= \sigma(u)|\nabla\varphi|^2 && \text{in } \Omega_T = \Omega\times(0,T),\\ \nabla\cdot(\sigma(u)\nabla\varphi) &= 0 && \text{in } \Omega_T\\ u = 0,\quad \varphi &= \varphi_0 && \text{on } \Gamma_T = \partial\Omega\times(0,T),\\ u(\cdot,0) &= u_0 && \text{in } \Omega, \end{aligned}$$

where Ω, the domain occupied by the electrical device, is an open, bounded and smooth enough subset of $\mathbb{R}^N$, $N \geq 1$ and $T > 0$. The nonlinear source term $\sigma(u)|\nabla\varphi|^2$ is the Joule effect.

The purpose of this work is to establish the existence of a certain class of solutions to this system under certain weak assumptions on data. The fundamental obstacle in the resolution of this problem lies in the degenerate character of the parabolic equation ($a(0) = 0$, $a(s) > 0$ for all $s \neq 0$) and the non-uniformly elliptic character of the elliptic equation ($\sigma(s) > 0$ for all s,). In that case, the existence of weak solutions are not guaranteed, and we have to deal with another type of solutions, namely, capacity solutions. This situation covers those cases of practical interest, for instance, when $a(s)$ is given by the Wiedemann–Franz law, $a(s) = Ls\,\sigma(s)$ for some constant value $L > 0$, and with metallic conduction; that is, $\sigma(s) = \mathrm{O}(s^{-1})$ for $|s| \gg 1$.

Modelling, analysis and simulation of case hardening. **Lucia Panizzi** (Scuola Normale Superiore di Pisa, Italy) IC/MT1880/152

A mathematical model for the gas carburizing in steel is presented. Carbon is dissolved in the surface layer of a low-carbon steel part at a temperature sufficient to render the steel austenitic, followed by quenching to form a martensitic microstructure. We have a nonlinear evolution equation for the temperature, coupled with a nonlinear evolution equation for the carbon concentration, both coupled with two ordinary differential equations to describe the phase fractions. The coupling between the heat and the carbon diffusion part of the model is given through the temperature-dependent carbon diffusivity coefficient on the one hand and through the source term in the carbon equation on the other hand, depending implicitly on carbon and temperature through the phase fractions. We present mathematical results concerning the well-posedness of the model and finally present a simulation of the process using a finite element approximation.

IC/MP623/015: Mathematics for steel manufacturing. #2

Organiser: Dietmar Hömberg (Weierstraß-Institut Berlin, Germany)
Co-organiser: Michael Wolff (Universität Bremen, Germany)

(For abstract, see session #1 above.)

Optimal control of a thermo-mechanical model of phase transitions in steel. **Daniela Kern** (Weierstraß-Institut Berlin, Germany), Dietmar Hömberg (Weierstraß-Institut Berlin, Germany) IC/MT1740/152

We consider an optimal control problem concerning heat treatment of steel.

The mathematical model consists of the equations of thermoelasticity coupled to a system of rate laws accounting for the phase transition kinetics. For the coupling a mixture ansatz for the different thermal expansion coefficients is used. In contrast to classical thermoelasticity this leads to residual deformations whenever the resulting phase distribution at end-time is inhomogenous.

We show well-posedness of the mathematical model, investigate the optimal control problem and conclude with some numerical simulations.

Optimization of induction heat treatment process for steel parts . **Francois Bay** (Ecole des Mines de Paris, France) IC/MT3465/152

Induction heating is being increasingly used for heat treatment of steel parts. These processes aim mostly at achieving a certain level of hardness for the final part. Heat treatment processes often require aiming at a precise path in space and time for temperature evolution.

We shall present here a specific optimization procedure, coupled to a numerical model for induction heat treatment processes for steel parts.

The direct induction heating model [1] solves both Maxwell equations as well as the heat transfer equation, using a finite element-based space discretisation, which leads to a coupled system of equations for the electromagnetic and heat transfer computations. This coupled system provides the constraints of our optimization problem.

We use a conjugate gradient type method for minimizing the cost function. Once the descent direction has been computed, the descent-step is used to get the value of the cost function as small as possible through a parabolic interpolation algorithm.

The computation of the cost function sensitivity with respect to the control parameters is based on an optimal control approach. We define the Lagrangian of the problem. After some mathematical treatment of equations [2], we then get the adjoint thermal field and the adjoint electromagnetic field.

Results will be presented on heat treatment cases for which we aim at improving frequency, current density and inductor velocity.

References

1 F. Bay, V. Labbe, Y. Favennec,J.L. Chenot, A numerical model for induction heating processes coupling electromagnetism and thermomechanics, International Journal for Numerical Methods in Engineering, Vol 58, pp 839-867, 2003

2 Y. Favennec, V. Labbe, Bay F., Induction heating process optimization: a general optimal control approach, Journal of Computational Physics, 187, 68-94, 2003

Control of laser surface hardening . **Wolf Weiss** (Weierstraß-Institut Berlin, Germany) IC/MT1230/152

Several control strategies for the laser surface hardening of steel are discussed. The goal is to achieve a prescribed hardening depth avoiding surface melting. The mathematical model consists of a system of ODEs for the phase fractions coupled with the heat equation. The system is solved semi-implicitely using the finite element method. To obtain a uniform hardening depth the first attempt is to use PID control to achieve a constant temperature in the hot spot of the laser beam on the surface. However, the numerical results prove that this is not sufficient. The best strategy is to control the temperature close to the lower boundary of the hardening zone. Then one can compute the optimal temperature in the hot spot of the beam and use it as the set-point for the pyrometer control of the real process.

Constrained optimization of laser welding models. **Jonathan Montalvo Urquizo** (Universität Bremen, Germany), Alfred Schmidt (Universität Bremen, Germany) IC/MT1839/152

The laser welding process depends not only in the nature of the material to be welded, but also in diverse welding parameters like velocity, laser type and strength, etc. During the weld creation, the material pieces are exposed to high temperature changes in a very short period of time. This fast changes can result in high residual stress and consequently in mechanical disadvantages for the welded piece (e.g. hot cracks, loss of strength, etc.).

In order to reduce these disadvantages, the search for the best calibration of the welding parameters is of interest. We present a simplified model for laser welding simulation coupled with an optimization procedure to find some of the parameters that better suit to the aims of small residual stresses, narrow welds, high welding speeds and low laser power.

The optimization is based in a reflective trust region procedure for nonlinear constrained problems and the weld simulations are implemented in ALBERTA.

This talk reports the work done within the graduate school Scientific Computing in Engineering as a joint computational and experimental project between the *Zentrum für Technomathematik* and the *Bremer Institut für angewandte Strahltechnik*.

IC/MP209/153: Numerical methods for chemically reacting flows.

Organiser: Jeffrey Banks (Sandia National Laboratories, USA)
Co-organiser: John Shadid (Sandia National Laboratories, USA)
Co-organiser: Donald Schwendeman (Rensselaer Polytechnic Institute, USA)

Chemically reacting flows are important to many industrial applications. These applications are wide ranging and include convectively dominated flows such as detonation waves in high explosives, laminar and turbulent combustion systems, and diffusively dominated flows in devices such as chemical vapor deposition (CVD) reactors. Numerical methods for the simulation of such wide ranging phenomenon are necessarily quite different, but many of the underlying principles are common throughout. The goal of this mini-symposium is to bring together scientists working in these different fields and to provide a broad overview of numerical methods and simulation results for this wide range of combustion problems.

A posteriori *error estimation for flamelet models.* **Pascal Turbis** (Université de Montréal, Canada), Anne Bourlioux (Université de Montréal, Canada), Alexandre Ern (École Nationale des Ponts et Chaussées, France) IC/MT1936/153

Flamelets are asymptotic solutions for the full transport of reactants in the limit of very thin flames. The objective here is to estimate the modelling errors when flamelets are used as turbulent closure, including cases with moderately thin flames. The challenge is to perform such estimation on the go, at a computational cost not exceeding significantly that of using flamelet libraries. We show this can be accomplished using the *a posteriori* error estimators introduced by Braack and Ern. So-called adjoint flamelet libraries are used to estimate errors, with application to model selection within a hierarchy of models, or parameter optimization for a given model.

An overview of the application of fully-coupled Newton-Krylov solution methods for FE simulation of transport/reaction systems. **John Shadid** (Sandia National Laboratories, USA), Roger Pawlowski (Sandia National Laboratories, USA), Paul Lin (Sandia National Laboratories, USA), Andrew Salinger (Sandia National Laboratories, USA) IC/MT2575/153

The need to simulate fluid flow systems with thermal energy and mass species transport, along with non-equilibrium chemical reaction is common in advanced technology applications. These systems are strongly coupled, highly nonlinear and characterized by multiple physical phenomena that span a very large range of length and time scales. These characteristics make the scalable, robust, accurate, and efficient computational solution of these systems extremely challenging.

In this presentation I will overview a number of the important solution methods that our research group has applied in the large-scale simulation of transport/reaction systems. The solution methods that we employ include, fully-implicit time integration, direct-to-steady-state solution methods, continuation, bifurcation, and optimization techniques. The resulting large sparse linear systems that are generated by these methods are solved by the application of parallel preconditioned Newton-Krylov methods. The preconditioners include additive Schwarz domain decomposition (DD) and multi-level preconditioners.

To demonstrate the capability of these methods I will present simulation and performance results for a range of representative low heat release and high heat release transport / reaction simulations.

*This work was partially funded by the Department of Energy's Mathematical, Information and Computational Sciences Division, and was carried out at Sandia National Laboratories operated for the U.S. Department of Energy under contract no. DE-ACO4-94AL85000

A fully-implicit FE formulation for plasma/transport-reaction and resistive magneto-hydrodynamic systems. **Roger Pawlowski** (Sandia National Laboratories, USA), John Shadid (Sandia National Laboratories, USA), Jeffrey Banks (Sandia National Laboratories, USA), Pavel Bochev (Sandia National Laboratories, USA) IC/MT2493/153

Plasma systems with strong electro-magnetic effects and chemical species transport and reaction occur frequently in nature and are critical for many important technological applications. Examples include stellar interiors, gaseous nebula, the earth's magnetoshpere, and Tokamak and Z-pinch physics. These systems are described by a set of partial differential equations that conserve momentum, mass, charge, and energy for chemical species along with Maxwell's equations for the electric and magnetic fields. The resulting equations are strongly coupled, highly nonlinear, and span a large range of time and length scales, making the scalable, robust, and accurate solution of such systems extermely challenging.

In this presentation, we will discuss the initial development of a new PTR/MHD formulation based on unstructured finite element methods and fully implicit time intergration techniques. Our initial implementation employs a variational multi-scale stabilized finite element solver that implicitly enforces div B = 0 by use of a vector potential formulation. We will discuss numerical performance, accuracy, and scalability. Example problems will include fast magnetic reconnection and DC plasma arc jets.

*This work was partially funded by the DOE Office of Science AMR Program, and was carried out at Sandia National Laboratories operated for the U.S. Department of Energy under contract no. DE-ACO4-94AL85000

IC/MP209/153: Numerical methods for chemically reacting flows. #2

Organiser: Jeffrey Banks (Sandia National Laboratories, USA)
Co-organiser: John Shadid (Sandia National Laboratories, USA)
Co-organiser: Donald Schwendeman (Rensselaer Polytechnic Institute, USA)

(For abstract, see session #1 above.)

Simulation of lean pre-mixed turbulent combustion. **John Bell** (Lawrence Berkeley National Laboratory, USA) IC/MT1482/153

Both environmental and economic concerns have generated significant interest in developing new fuel-flexible combustion systems that can employ alternative fuels such as hydrogen, ethanol or syngas. Effective utilization of these fuels requires combustion devices that can operate cleanly and efficiently over a broad range of fuels and fuel mixtures. Lean-premixed systems have the potential for meeting these requirements; they operate at high efficiency and have low NOx emissions due to reduced burnt gas temperatures. Although traditional scientific approaches based on theory and laboratory experiment have played essential roles in developing our current understanding of premixed combustion, they are unable to meet the challenges of designing fuel-flexible lean, premixed combustion devices. Computation, with its ability to deal with complexity and its unlimited access to data, has the potential for addressing these challenges. Realizing this potential requires the ability to perform high fidelity simulations of turbulent lean premixed flames under realistic conditions. Estimates of the computational cost of such simulations suggest that naive simulation approaches would be prohibitively expensive. In this talk, we examine the specialized mathematical structure of combustion problems and discuss approaches to

simulation that exploit this structure. Using these ideas we can reduce computational cost by three to four orders of magnitude, making it possible to perform high-fidelity simulations of realistic laboratory flames. We will illustrate this methodology by considering several configurations to illustrate the methodology and discuss how this type of simulation is changing the way researchers study combustion.

Detonation evolution and structure for a model of reactive two-phase flow. **Donald Schwendeman** (Rensselaer Polytechnic Institute, USA), Ashwani Kapila (Rensselaer Polytechnic Institute, USA) IC/MT1710/153

A two-phase model of heterogeneous explosives is examined computationally by a new numerical approach that is a modification of the standard Godunov scheme. The approach generates well-resolved and accurate solutions using adaptive mesh refinement, and treats rationally the nozzling terms that render the otherwise hyperbolic model incapable of a conservative representation. A broad range of the parameter space is considered and two possible structures of steady, planar detonations are identified, along with subregions of the parameter space where they exist. The transient processes subsequent to impact by a low-speed piston are discussed, and these show the transition from a compaction wave to one or the other of the two steady detonation waves. Two-dimensional evolution for problems of detonation diffraction are also discussed.

Simulations of compliantly confined, shock-desensitized high explosives. **Jeffrey Banks** (Sandia National Laboratories, USA) IC/MT1731/153

High explosive charges are used in many industrial and laboratory settings. The detonation mechanism involved in such charges are quite complex and many questions involved in their modeling and simulation remain open. Here we present a model for shock desensitization of a high explosive and place this in the context of a multi-material flow solver. This solver is a high-resolution Godunov method which operates on a collection of overset grids and uses adaptive mesh refinement (AMR) to capture small scale features within the flow. The multi-material capability is used to model the compliant confinement of a high-explosive charge by air, brass, or some other relevant material. The effects of this confinement then couple with the shock desensitization model within the explosive. The result is a simulation tool which can more accurately reproduce experimental evidence. We present a number of examples including detonation diffraction around corners and detonation failure in converging rate sticks. These results are compared to results obtained using rigid confinement and/or without any shock desensitization model.

IC/MP148/154: Multiscale problems in materials sciences.

Organiser: Christof Eck (Universität Erlangen–Nürnberg, Germany)
Co-organiser: Peter Knabner (Universität Erlangen–Nürnberg, Germany)

Micro- and nano-structures are an indispensable tool in the engineering of new advanced materials. They arise in the production process of materials (as e.g., the production of metals by casting processes), or the production of semiconductor devices by epitaxy, and they are relevant for many important phenomena; e.g., the shape memory effect in shape memory alloys, the evolution of plastic deformations by slip lines, and magnetism.

Up-to-now, the research on micro- and nanostructures has mainly adressed models on a single scale. On one hand, there are completely avaraged or homogenized models for processes having a technologically relevant scale; where the properties of micro- or nanostructures enter only in a very heuristic way via macroscopic constitutive laws. On the other hand, there are specialized models for the evolution of single microstructure elements (as e.g., single dendrites in casting processes), single or few slip lines in plastic deformation, single or few molecules in MD simulations. These techniques are typically applicable to very small length and/or time scales only.

In the recent years, new analytical and computational techniques arose that promise to bridge large scale differences and therefore enable the simulation of micro- and nanostructures within length scales of technical relevance. Prominent examples are the heterogeneous multiscale method, and the multi-scale FEM, as well as advances in more traditional areas as homogenization.

The aim of the minisymposium is to present the latest development concerning the coupling of different models and different scales and to discuss and compare the different mathematical and computational concepts.

The interplay of thermodynamics and kinetics in crystal growth. **Axel Voigt** (FZ caesar, Germany) IC/MT983/154

We discuss a meanfield model for a one-dimensional step in which a detailed atomistic structure is considered. The model consists of a diffusion equation for an edge-adatom density on the evolving step, a convection equation for a kink density on the step and a velocity law for the evolution of the step. The equations are coupled through atomistc processes, such as attachment/detachment of edge-adatoms at kinks, nucleation/destroying of kink-dimers and so on. The resulting multiscale model requires besides the step stiffness only atomistic hopping rates as parameters. The stiffness is computed from atomitic models. We introduce a finite element discretization and show results for thermodynamic smooting, kinetic smoothing and an instability resulting from a kink Ehrlich-Schwoebel barrier.

Two-scale modeling of adsorption processes at structured surfaces. **Heike Emmerich** (RWTH Aachen, Germany), Maria Radke de Cuba (RWTH Aachen, Germany), Sibylle Gemming (RWTH Aachen, Germany), Gudrun Schuerer (RWTH Aachen, Germany) IC/MT1856/154

We investigate the adsorption behavior of oxalate on a structured glass surface at several temperatures. For this purpose a hybrid scheme was developed which combines a two-dimensional anisotropic Ising model mapped on a lattice gas model with a phase-field model for vicinal surface growth. The microstructure dynamics on the vicinal surface are calculated using the phase-field method which is based on the classical Burton-Cabrera-Frank (BCF) theory. The molecular behavior of individual adatoms is resolved by the Monte-Carlo generated dynamics of the Ising model which include an incoming flux, diffusion and desorption. The corresponding constants measured by Monte-Carlo simulation are put into the phase-field part. During Monte-Carlo simulation the particles form clusters or attach to the step edges. To each cluster a binding energy is assigned which is inherited from the Ising Hamiltonian. Depending on this energy it is decided if the corresponding cluster becomes part of the surface after the transformation to the phase-field part. Therefore the atomic and micro-scale dynamics influence each other dynamically during surface evolution by an Arrhenius-like reaction path. The corresponding energy scales are derived by first principle calculations. Several growth modes are distinguished in the present scheme characterized by morphology and roughness which decreases with increasing temperature.

A finite-difference approach for concurrent multiscale computations in solids. **Shaoqiang Tang** (Peking University, PR China) IC/MT1802/154

In concurrent multiscale computations for solids, the atomistic computations capture detailed dynamics in a selected MD subdomain, while the macroscopic computations are performed in the vast surrounding region. Almost all existing multiscale methods adopt finite element approaches in the MC region, and usually use an approximated Hamiltonian for deriving the FEM schemes. A handshaking region is usually designed to reduce interfacial reflections. The approximation errors may not be easy to analyze and hard to control.

In this talk, we propose a class of velocity interfacial conditions and formulate a finite difference approach for multiscale computations of crystalline solids with relatively strong nonlinearity and large deformation [2]. With a coarse grid cast over the whole domain, we compute the coarse scale dynamics using finite difference schemes derived by a matching differential operator method [1], together with a reassignment by averaging the fine scale solution for the atomistic subdomain. In a coarse scale time step, we adopt a linear wave approximation around the interface, with the coefficients determined from the coarse grid solution. Based on this approximation, we develop a class of velocity interfacial conditions with different order of accuracy. The interfacial conditions are straightforward to formulate, easy to implement, and effective for reflection reduction in crystalline solids with strong nonlinearity. Multiscale simulations in one and two space dimensions demonstrate the accuracy, the robustness and the efficiency for the proposed approach.

[1] S. Tang, T.Y. Hou, W.K. Liu. A pseudo-spectral multiscale method: interfacial conditions and coarse grid equations. J. Comput. Phys., 213 (2006), 57-85.

[2] S. Tang. A finite difference approach with velocity interfacial conditions for multiscale computations of crystalline solids. Preprint.

A two-scale model for liquid phase epitaxy. **Christof Eck** (Universität Erlangen–Nürnberg, Germany) IC/MT1299/154

Liquid phase epitaxy is a special technique to grow thin solid layers from a liquid solution. The main mechanism is the deposition of atoms in monoatomar layers. Often epitaxy leads to microstructures of the phase interface that may be of technical relevance. We study a model for liquid phase epitaxy that consists of differential equations for the transport of fluid and solute in the liquid phase and a Burton Cabrera Frank (BCF) model for the growth of the solid layer. In order to derive a model that is suitable for a very small scale of the microstructures, we apply homogenization techniques and construct a two-scale model that couples macroscopic equations for the transport processes in the fluid to microscopic evolution equations for the solid phase. For a phase field approximation of the BCF model, the solvability of the two-scale model is analyzed and an estimate for the model error is derived. A possible extension of the model that incorporates the effect of elastic deformations in the solid phase will be given.

IC/MP148/154: Multiscale problems in materials sciences. #2

Organiser: Christof Eck (Universität Erlangen–Nürnberg, Germany)
Co-organiser: Peter Knabner (Universität Erlangen–Nürnberg, Germany)

(For abstract, see session #1 above.)

Minimizing the stray-field energy in micromagnetics subject to a convexified point-wise constraint. **Carsten Carstensen** (Department of Mathematics Humboldt-Universität, Germany), Dirk Praetorius (TU Wien, Austria) IC/MT3326/154

The large body limit in the Landau–Lifshitz equations of micromagnetics yields a macroscopic model without exchange energy and with convexified side conditions for the macroscopic magnetisation vectors. Its Euler Lagrange equations **(*P*)** read: Given a magnetic body $\Omega \subseteq \mathbb{R}^d$, $d = 2, 3$, an exterior field $\mathbf{f} \in L_2(\Omega)^d$, and the convexified anisotropy density $\phi^{**} : \mathbb{R}^d \to \mathbb{R}_{\geq 0}$, find a magnetization $\mathbf{m} \in L_2(\Omega)^d$ and a Lagrange multiplier $\lambda \in L_2(\Omega)$ such that a.e. in Ω

$$\nabla u + D\phi^{**}(\mathbf{m}) + \lambda \mathbf{m} = \mathbf{f},\ |\mathbf{m}| \leq 1, \quad \lambda \geq 0,\ \lambda(1 - |\mathbf{m}|) = 0.$$

The potential $u \in H^1_{\ell oc}(\mathbb{R}^d)$ solves the (Maxwell) equations

$$\nabla u \in L_2(\mathbb{R}^d)^d \text{ and } \operatorname{div}(-\nabla u + \mathbf{m}) = 0 \text{ in } \mathcal{D}'(\mathbb{R}^d)$$

in the entire space. It therefore appears natural to recast the associated far field energy into an integral operator $\mathcal{L}$ which maps $\mathbf{m}$ to the corresponding potential u.

The proposed numerical scheme involves the operator $\mathcal{L}$ and replaces the pointwise side-condition $|\mathbf{m}| \leq 1$ by a penalization strategy. Given a triangulation $\mathcal{T}$, the induced space of piecewise constant functions $P_0(\mathcal{T})$ on Ω, and a penalization parameter $\varepsilon > 0$, the discrete penalized problem **($P_{\varepsilon,h}$)** reads: Find $\mathbf{m}_h \in P_0(\mathcal{T})^d$ such that for all $\boldsymbol{\nu}_h \in P_0(\mathcal{T})^d$

$$\langle \nabla(\mathcal{L}\mathbf{m}_h) + D\phi^{**}(\mathbf{m}_h) + \lambda_h \mathbf{m}_h ; \boldsymbol{\nu}_h \rangle_{L_2(\Omega)} = \langle \mathbf{f} ; \boldsymbol{\nu}_h \rangle_{L_2(\Omega)}$$

with $\lambda_h := \varepsilon^{-1} \dfrac{\max\{0, |\mathbf{m}_h| - 1\}}{|\mathbf{m}_h|} \in P_0(\mathcal{T})$.

Numerical aspects addressed in the presentation include the integration of the matrices with quadrature rules and hierarchical matrices as well as a priori and a posteriori error control with a reliability-efficiency gap and adaptive mesh-design.

Discrete-to-continuum limit of the magnetic force between rigid bodies dependent upon their distance. **Anja Schlömerkemper** (Max-Planck-Institut Leipzig, Germany), Bernd Schmidt (California Institute of Technology, USA) IC/MT1677/154

In earlier work[1,2], the discrete-to-continuum limit of the magnetic force between two bodies being in contact was studied and a new lattice dependent term was found. In order to obtain a better understanding of magnetic forces at small distances between rigid magnetic bodies, we consider an analogous problem: we study the magnetic force between two bodies which are assumed to be a distance apart on the lattice scale but in contact on the scale of the continuum. In the continuum limit we obtain an additional term which depends on the distance between the two bodies on the lattice scale. We discuss analytical properties of this additional term.

[1] Schlömerkemper, A.; Mathematical derivation of the continuum limit of the magnetic force between two parts of a rigid crystalline material. *Arch. Rational Mech. Anal.* **176** (2005), pp.227–269.

[2] Popović, N., Praetorius, D. and Schlömerkemper, A.; Analysis and numerical simulation of magnetic forces between rigid polygonal bodies. Part I: Analysis. MPI für Mathematik in den Naturwissenschaften, Leipzig, Preprint 63/2006.

The effect of defects on the motion of a martensitic phase boundary. **Patrick Dondl** (California Institute of Technology, USA) IC/MT2634/154

We study the role of defects in the quasistatic evolution of a martensitic phase boundary. Martensitic phase transformations involve a change in shape of the underlying crystal, and thus the propagation of the phase boundary is accompanied by an evolving mechanical stress and strain field. This gives rise to a nonlocal free boundary problem, one where the evolution of the free boundary is coupled to a partial differential equation. Often, real materials contain defects which can potentially pin the interface and contribute to the hysteresis, and understanding this is the goal of this work. We present a mathematical model and a proof of existence in the sense of sets of finite perimeter. We then present numerical simulations and analysis of both the fully nonlocal problem as well as a linearized version, and draw conclusions on the role of defects on hysteresis.

A phase field model in electro-wetting and related phenomena. **Marco Fontelos** (Universidad Autónoma de Madrid, Spain), Christof Eck (Universität Erlangen–Nürnberg, Germany), Günther Grün (Universität Erlangen–Nürnberg, Germany) IC/MT4588/154

Electro-wetting phenomena involve films of viscous fluids over solid substrates, in the present of electric fields and with moving electric charges. This yields a system of equations for the charge density, electrostatic potential and velocity field together with forces due to surface tension and electrostatic repulsion between charges of the same sign. We develop a description of the fluid interface through a phase field satisfying a convective Cahn–Hilliard equation and present a thermodynamically consistent deduction of the model consisting of Stokes equations and advection-diffusion equations for the motion of charges coupled with it. We provide a mathematical proof of global existence of weak solutions to the model and discuss the implementation of numerical methods to solve it.

IC/MP39/154: Simulation in nano-technology and bio-mathematics.

Organiser: Leela Rakesh (Central Michigan University, USA)

Understanding the mathematical rigorness is very crucial for any minute details in nanotechnology and its social impact. The symposium on nanomathematics is to support the emerging nanotechnology and nanoscience revolution through an interdisciplinary mathematical modeling and simulation applied to the understanding of biology, chemistry and physics of nanomaterials. We will discuss some of the recent advances and publications by myself and colleagues working closely with Chemist, Doctors, Engineers, and Industrialists in this area.

The US Department of Energy has identified a key potential research target for future development of the field: "lack of development of theory, analytical techniques, and modeling and simulation tools (TAMS)". A collaborative effort by some selected universities in US and industries would address these issues by developing a coherent, yet multidisciplinary, program in the fundamentals of TAMS at the nanoscale and in the problems of linking behaviour on the small scale to the large scale. In addition to being truly active in the worldwide scene of nanoscience and nanotechnology education and research, it can potentially have an important, and possibly crucial, impact on the development of related commercial enterprises in the US. For example, the electronics industry will not risk deploying billions of devices based on molecular electronics, unless they are thoroughly understood and manufacturing processes are made predictable and controllable.

This symposium will contribute to the basic understanding of fluid dynamics and better analytical techniques, thus enabling the better design, modeling, predictability, efficiency and control of systems that involve fluids and will also address innovative uses of fluids in materials development, manufacturing, biotechnology, nanotechnology, clinical diagnostics and drug delivery. Another example related to the impact of nanotechnologies on the fluid and molecular dynamics, are highlighted by micro fluidics and the hybrid continuum molecular emergence as an enabling technology, and hence used in practical fluid and molecular dynamics problems from laminar flow control in aerospace applications to problems in medicine, thermodynamics and production engineering. For example,

(i) Complex Fluids: Rheology, instability, physics of polymer solutions, DNA, Molecular Dynamics simulations;
(ii) Micro- Nano- Bio- Fluid Mechanics: Micro fluidics, biomedical micro devices, Atomic force microscopy, Nuclear magnetic resonance, effects of nanoscale inclusions on rheological properties, flows in biomedical assistive devices, multiscale modeling of biological flow processes.

Nanoscale effects are also crucially important in the development of new materials such as the complex composites used in the aerospace industry, biomedical engineering for prosthesis to heart valves, Organometallic drug encapsulation for various cancer treatment and the revolution in communications technology promised by photonic optical fibers. Because TAMS has been identified as an enabler of nanoscience and technology, it could potentially have a great impact on the development of commercial enterprises in this area. Indeed, the uniqueness of this proposed activity could actually encourage and attract potential startup companies to the region.

Packing cylinders on a cylinder with contact constraints. **Eric Goold** (Central Michigan University, USA) IC/MT3563/0

The problem of cylinder packing is investigated. The specific problem is to determine the maximum number of congruent cylinders that can be packed around a core cylinder of arbitrary dimensions. The constraint is that their circular face must keep in contact with the core cylinder and there may be no overlapping. Only right circular cylinders are considered. Mathematically, a lower and upper bound is determined. A quantitative result is also found using a modified genetic algorithm. The algorithm was found to reproduce the published results for the top and bottom circular faces of the core which reduces to the problem of packing congruent circles within a circle. Several other algorithms are discussed along with their computational speeds.

Two-level atoms: normal-form approach. **Raghu Gompa** (Jackson State University, USA) IC/MT3700/0

Perturbation theory that is based on normal form techniques is studied in the context of Schrödinger initial value problem associated with two-level atoms to arrive at approximations that deviate in norm from the exact solution by a term of order e2t.

Differential geometry and the red blood-cell. **Wescott Vayo** (University of Toledo, USA) IC/MT3795/0

The usual mathematical expressions for the shape of the red blood cell, whether in rectangular or polar coordinates, are very complicated and difficult to use analytically. The main difficulty that remains unsolved is that related to the complexity of the mathematical expressions describing quantities of geometric interest. We have found that by using parametric equations and hyperbolic functions to describe the cell functioning are much easier. The usual differential geometric concepts of a normal red blood cell can be adopted to find interesting new formulas by incorporating ideas like FickŠs Law, etc.

Experimental and computational characterization of nanoscale dendritic organoplatinum antitumor drugs. **Bob Howell** (Central Michigan University, USA), Leela Rakesh (Central Michigan University, USA) IC/MT3858/0

Organo-platinum compounds exhibit broad antitumor activity. Cisplatin [cis-dichlorodiammine platinum (II)] is the most prominent of this family and is currently the most prescribed cancer drug. It is widely used for the treatment of human testicular, ovarian, bladder, head and neck carcinomas. However, it is an extremely toxic compound and side effects such as nephrotoxicity and myelotoxicity are major drawbacks for its use in clinical applications. A way to combat the side effects associated with the administration of platinum drugs would be to generate a prodrug conjugate that, when present in the extracellular fluid, would slowly release active platinum species at a level below the threshold for side effects. Traditionally, linear hydrophilic polymers have been examined for potential application as carrier platforms for these drugs. The advent of dendrimers, which are highly branched macromolecules with precisely controlled nanoscale size, shape and end-group functionality, has provided an excellent opportunity to design and formulate novel multivalent time-release drug systems. A program to do this is well-underway. For example, treatment of a generation 4.5 (carboxylate surface) poly(amidoamine) [PAMAM] dendrimer with diaquo(1,2-diaminocyclohexene) platinum(II) generates a nanoparticle with forty platinum moieties attached at the surface [D. Fan, B.A. Howell and L. Rakesh, Polym. Mater. Sci. Eng., 93, 946 (2005); B. A. Howell, D. Fan and Leela Rakesh, J. Therm. Anal. Cal., 85, 17 (2006)]. This polymer-drug conjugate displays a very good release profile for the platinum species. Under physiological conditions about 80

IC/MP39/154: Simulation in nano-technology and bio-mathematics. #2

Organiser: Leela Rakesh (Central Michigan University, USA)

(For abstract, see session #1 above.)

Modeling and simulation of the evolution of crystal morphologies with anisotropic surface free-energy. **Wen Zhang** (Oakland University, USA), Ian Gladwell (Southern Methodist University, USA) IC/MT3165/0

We present a mathematical model and computational method for the evolution of crystal surface by surface diffusion with anisotropic surface free energy. Employing the model and computation we study the evolution path of a single crystal to equilibrium and the morphologies of periodic surfaces. We examine examples of simple cubic crystals with different levels of anisotropic surface free energies and different initial configurations. The simulation results are compared with the atomic force microscopy studies of grain surfaces in annealing processes such as thermal grain-boundary grooving. The evolution is governed by a nonlinear 4th order time dependent partial differential equation. We find that with a mildly anisotropic surface free energy, the crystal morphology is smooth and evolves to a unique equilibrium crystal shape (ECS). In the cases of grain boundary grooving, the groove profiles are self-similar in the evolution and follow a power law with the exponent 1/4. However, the shapes of these profiles have striking differences from those developed under isotropic surface free energy. With a severely anisotropic surface free energy, depending on the initial crystal configuration and surface free energy, edges, corners and faceting by hill-and-valley structures on crystal surface may occur. A large planar surface facet in the ECS can be obtained, arbitrarily closely, using smooth anisotropic surface free energies. And a polyhedron Wulff shape is the limit of Wulff ECS with smooth anisotropic surface free energies. In general, the ECS reached in computation depends on the initial surface configuration. This dependence becomes more evident as the anisotropy becomes more severe but is less likely to occur for 3D crystals than for 2D crystals. By enforcing a corner condition in the cases of 2D crystals, we obtain better stability in the evolution, which leads to the ECS having lower total surface free energies than those obtained without satisfying the corner condition.

Molecular-dynamics simulation of PAMAM dendrimer–fullerene conjugates. **Leela Rakesh** (Central Michigan University, USA) IC/MT3220/0

We describe an attempts at preparing polyamidoamine (PAMAM) dendrimer-fullerene (C60) conjugates, using increasing generations (G0 to G4) of PAMAM and C60 in pyridine. Based on the synthesis of the PAMAM (G4)-C60 conjugate in a molar ratio of 1:30, Jensen etal had hypothesized that two surface amine group interact with one fullerene molecule to form the conjugates. Computer simulation study on the same system was to found to be excellent agreement based on the energy minimization process. The same computational techniques were then used to determine the energy-minimized structure of the remainder of the conjugates, and compare their solubility behaviors in pyridine along with (G4)-C60. The findings allow for a better understanding of structure-property relationships of these nano-hybrid materials, through investigation of the molecular shape, radial distribution function, and radius of gyration. Our findings reported herein may lead to improved syntheses of fullerene-dendrimer conjugates of various sizes as well as further understandings of their nanoscopic structures and topographical influences.

Complexation of PPI dendrimers with Zn(II) *ions.* **MInghui Chai** (Central Michigan University, USA) IC/MT3363/0

PPI [poly(propyleneimine)] dendrimers are multidentate ligands which can chelate with metal ions to form complexes using the primary and tertiary amino groups in their structures. In this study we used NMR spectroscopy to probe the preferred binding sites of different generation (G1–G3) PPI dendrimers with Zn(II) ions. AFM (atomic force microscopy) was also used to detect the sizes of these dendrimer-metal complexes as well as to explore their surface morphology. The results from the NMR study clearly show that Zn(II) ions prefer to chelate with the primary and tertiary amino groups on the exterior of the dendrimer. For a 1:8 ratio of the PPI–3/Zn(II) complex, interestingly all eleven unique protons can be well resolved in the 2D COSY spectrum. Based on the resolved 1H resonances, the 13C NMR resonances can be unambiguously assigned using 2D 1H13C HMQC experiments. In addition, the AFM study shows that the surface of the PPI–Zn(II) complexes is *harder* than the surface of the PPI dendrimers, which also indicates that the coordination between the dendrimer and the Zn(II) ion mainly occurs on the exterior of the dendrimer. Furthermore, the results from molecular dynamics simulations and ab initio calculations on the complexes of a different generation PPI dendrimers with Zn(II) ions are consistent with the conclusions from NMR studies. Therefore this work provides an insightful view of where and how metal ions bind with the dendrimers.

Skin, a smart hydrogel, and its nano-technological mimics. **Anja Mueller** (Central Michigan University, USA) IC/MT3481/0

Skin is the ultimate smart material that can turn chemical energy into mechanical energy and heat. It fulfills a variety of vital functions for the body under various operating conditions and it respond to changing environments. It is a hydrogel with multiple components, regulated by only a few general regulation and transport mechanisms. In this talk the structure and function of major components of skin as a hydrogel are presented, as well as the basic regulation mechanism. This information can be used for numerical simulation of the steady-state deformation and regulation of a smart hydrogel under an external field. Nanotechnological mimics of some of these structures and regulation mechanisms are then compared with skin itself. Such investigation will lead to the discussion of skin scaffolds for burn victims that include the majority of functions of skin, allowing for improved healing of extensive burns.

IC/MP215/154: Multiscale porous media: applications.

Organiser: Mary Wheeler (University of Texas at Austin, USA)
Co-organiser: Hector Klie (University of Texas at Austin, USA)
Co-organiser: Robert Scheichl (University of Bath, UK)

Multiphase flow, transport, and reaction in porous media have important applications in petroleum reservoir engineering and in groundwater flow. These often involve multiphase multiphysics processes across multiple temporal and spatial scales whose discretisation leads to large highly ill-conditioned linear systems. This minisymposium showcases recent advances in applications, with emphasis on reservoir simulation, multiphase flow, and transport of contaminants in heterogeneous media. It is linked to the two other minisymposia: “Multiscale porous media: discretizations” and “Multiscale porous media: solvers”.

Multiscale time stepping for contaminant transport in an heterogenous medium. **Jean Roberts** (INRIA Rocquencourt, France), Jérôme Jaffré (INRIA Rocquencourt, France), Estelle Marchand (INRIA Rocquencourt, France), Amel Sboui (INRIA Rocquencourt, France) IC/MT2931/154

The problem of simulating flow and transport of radionuclides in a neighborhood of an underground nuclear waste storage site is very complex due in large part to the widely varying scales involved in the physical model. The storage site itself, the source of the contaminants, is heterogeneous and of complex geometry. The far field, the area surrounding the storage site is of much larger dimension, roughly 50 kilometers by 50 kilometers in horizontal extent and 500 meters in depth and is also very heterogeneous. The physical properties of the various geological layers differ greatly yielding permeability, diffusion, and dispersion coefficients that vary over several orders of magnitude. Thus the flow and transport in the different layers take place on different time scales. Further, since the half life of some of the radionuclides is quite long the simulation corresponds to a time duration of several hundred thousands of years.

In this presentation we show how subdomain time stepping may be implemented in order to use time steps appropriate to the time scales of the processes taking place in the different layers. The domain is divided into nonoverlapping subdomains respecting the geological layers. Different size time steps are used for advection and diffusion-dispersion and different size time steps are used in different layers. The diffusion-dispersion time steps are implicit and at time steps in which the global problem must be solved, domain decomposition is used. Numerical experiments will be presented.

Multiscale finite-element methods and adaptive coarsening: moving towards Earth Model reservoir simulation. **Jørg Aarnes** (SINTEF, Norway) IC/MT1101/154

Reservoir simulators normally take as input coarsened geological models derived through an upscaling process. However, partly due to grid-limitations, upscaled models generally fail to capture important subscale features, such as narrow high-flow channels and barriers, properly. The generation of simulation grids is also usually non-automated, and generally the most time-consuming part of the upscaling process. Due to limitations of upscaling, there is now a growing demand for Earth Model reservoir simulators capable of taking geostatistical models provided by geologists as input. If simulations are not to be performed on the initial grid, then all grid coarsening strategies should be fully automated, and designed to preserve the important subscale features in the geostatistical model. We propose combining a multiscale mixed/mimetic finite element method (MsMFEM) for computation of pressure and velocities with an automated, weakly constrained, adaptive grid coarsening strategy.

The MsMFEM provides accurate and detailed velocity fields at the cost of a flow-based upscaling methods, also for models with complex grid geometries, and puts almost no constraints on the coarsened grid used to discretize the pressure equation. As the grid constraints associated with upscaling is primarily related to discretization of the pressure equation, MsMFEM alleviates one of the main limitations of upscaling, and readily allows for automated coarsening strategies. In addition, by providing mass conservative velocity fields on an underlying fine grid, e.g., the geostatistical model, MsMFEM allows the use of grids for computing phase transport that are adaptive to fine-scale features. In our coarsening approach, the only grid constraints are that grid cells should be connected, have at least some minimum volume, and less total flow than some threshold. Results will be presented to demonstrate the general performance of the combined methodology.

Multiscale finite-volume method for three-phase flow in porous media. **Seong Lee** (Chevron ETC, USA), Christian Wolfsteiner (Chevron ETC, USA), Hamdi Tchelepi (Stanford University, USA) IC/MT1178/154

The multiscale finite volume (MSFV) method is extended to the standard black oil formulation for three phase, compressible flow (oil-gas-water) with gravity/capillarity. The mass transfer between oil and gas phases is described by solution gas. An operator splitting is employed to decompose the pressure equation into elliptic part, buoyancy/capillary force dominant part, and inhomogeneous part with source/sink (wells) and accumulation. Flow and transport equations are decoupled and solved sequentially. An accurate coarse grid operator is derived for the flow equation (pressure and velocity) and a local fine grid solution is reconstructed via basis functions. In addition, adaptive computation is extensively implemented for numerical efficiency. The MSFV method of black oil formulation allows us to study a large class of practical problems. The numerical efficiency of MSFV is analyzed and the robustness and computational efficiency of the MSFV is demonstrated by simulating large, heterogeneous reservoir models.

A multiscale method for parameter estimation in reservoir simulation. **Adolfo Rodriguez** (University of Texas at Austin, USA), Hector Klie (University of Texas at Austin, USA), Mary Wheeler (University of Texas at Austin, USA) IC/MT1616/154

The main objective of oil parameter estimation (history matching) is to find model parameters such that numerical predictions agree with past observed reservoir response. Once parameters are estimated, the reservoir model is employed to simulate future reservoir performance on a wide range of exploitation scenarios. However, history matching is a very challenging problem due to the ill-posedness and high computational cost involved in estimating hundreds of thousands to millions of parameters in conventional reservoir settings. These parameters are generally given by permeability values at each block of the spatially discretized domain. To effectively alleviate this problem, we introduce a multiscale approach in such a way that the parameter estimation is first performed at a coarse resolution scale and the results are then downscaled to be used as an improved initial guess for the original scale. This is accomplished by applying the Singular Value Decomposition (SVD) to the prior permeability field so that it is expressed as a weighted summation of an eigenimage basis. The SVD expansion ensures compatibility with previous geological nterpretations while gives flexibility to adjust the fine scale details of the model. An upscaling procedure based on wavelets is applied to the expansion in order to obtain a coarse-scale expansion whose weights are determined by a history matching procedure. Once the weights are estimated, they are downscaled and used along the original eigenimages to create a new initial guess for the fine-scale problem. The procedure can be repeated for a number of intermediate scales in order to facilitate the downscaling procedure. In order to capture finer details of the original parameter space, we release the SVD parameterization at the finer scale. In this way, the estimation is able to include permeability features at each grid-block. The above procedure is illustrated through a number of numerical experiments on reality-based datasets.

IC/MP652/155: Inverse problems and applications I: mathematical techniques for imaging.

Organiser: Oliver Dorn (Universidad Carlos III de Madrid, Spain)
Co-organiser: Manuchehr Soleimani (University of Manchester, UK)

New mathematical techniques are emerging in a variety of real world applications, for example in the broad area of imaging and inverse problems. The need for combining novel mathematical concepts with powerful and flexible numerical algorithms is ever increasing in this area. In the session, four specialists will present novel mathematical approaches for important real world problems from medical, industrial and geophysical tomography, such as diffuse optical tomography, microwave medical imaging, thermal conductivity and heat capacity tomography, and the characterization of nonconventional petroleum reservoirs.

A Newton–Krylov method for optical tomography. **Simon Arridge** (University College London, UK) IC/MT2912/155

Several problems in medical imaging can be characterised as parameter identification problems, and can be solved for example by an output least squares method. Newton schemes are amongst the most popular, and often involve construction of large dense Jacobian matrices that can be prohibitive to store. In this talk we present an efficient method for Gauss–Newton and full-Newton methods that do not involve the storage of the Jacobian. The method is shown applied to the recovery of absorption and scattering cross-sections in optical tomography.

Level-set techniques for microwave medical imaging. **Natalia Irishina** (Universidad Carlos III de Madrid, Spain), Oliver Dorn (Universidad Carlos III de Madrid, Spain), Miguel Moscoso (Universidad Carlos III de Madrid, Spain) IC/MT2904/155

Recently there has been increased interest in the use of microwaves for the early detection of breast cancer. The high contrast of electromagnetic parameters of malignant tissue with respect to healthy tissue makes this technique a very promising alternative to the more traditional technique of X-ray imaging which suffers from low contrast images and a potential health risk due to the ionizing nature of the probing radiation. However, there are still several mathematical problems to be resolved before microwave data can be used for the early diagnosis of breast cancer. In order to reliably detect and characterize a tumor in its early stage of development it is necessary to reconstruct from the data basic information about its location, its size, its shape and its electromagnetic parameter values. For example, an indication whether a tumor is benign or malign is given by the irregularity of its surface. Also the electromagnetic parameter values of the tumor can give important information about its nature. In our contribution we will present a novel technique for detecting and characterizing small tumors in the breast from microwave data which uses a level set representation of its shape. In particular, we focus on the simultaneous characterization of the shape, size and location of the tumor together with its electromagnetic properties. We present numerical examples in 2D in order to discuss the performance of our new technique in realistic situations.

Reconstruction of thermal conductivity and heat capacity using a tomographic approach. **Ville Kolehmainen** (Kuopion Yliopisto, Finland) IC/MT3019/155

We consider the estimation of the volumetric heat capacity and the thermal conductivity as distributed parameters. The measurement scheme consists of sequentially heating the boundary of the object in different source locations and measuring the induced temperature evolutions in different measurement locations on the boundary. The estimation of the distributions of volumetric heat capacity and thermal conductivity based on these boundary data is an ill-posed inverse boundary value problem. We propose an approach which is based on transient data on the boundary and the modelling of the unknown coefficients as Markov random fields. We propose a statistical (Bayesian) approach for this estimation problem. The intended applications are non-destructive retrieval of defects as well as the estimation of macroscopic characteristics of novel materials. We evaluate the proposed approach by a numerical simulation.

Shape-based techniques for an inverse two-phase flow problem in reservoir characterization. **Rossmary Villegas** (Universidad Carlos III de Madrid, Spain), Oliver Dorn (Universidad Carlos III de Madrid, Spain), Miguel Moscoso (Universidad Carlos III de Madrid, Spain), Manuel Kindelan (Universidad Carlos III de Madrid, Spain) IC/MT3006/155

Reservoir characterization is an important component nowadays in the petroleum industry for enhancing hydrocarbon production. Mathematically an inverse problem for multiphase flow in porous media needs to be solved for reconstructing physical fluid flow properties (for example permeability) of the reservoir. When a reservoir contains more than one rock-type (lithofacies), then standard inversion techniques are inappropriate since they yield oversmoothed reconstructions of the interfaces between regions of different rock-types. We propose in this talk a novel technique which is able to reconstruct simultaneously the boundaries of regions of different rock-types and the smoothly varying internal permeability structure inside of these regions. For describing the different lithofacies, a level set technique is employed. The reconstruction of the regions is done by an evolution of the level set function describing the individual lithofacies in a descent direction of a given cost functional. The internal permeability profiles are recovered by additional evolution laws for these quantities. Here we use two different strategies, a pixel-based representation and a parameterized representation of the permeability profile inside of each region. Using an efficient adjoint scheme, the calculation of descent directions for the shapes and the internal permeability profiles requires only one direct and one adjoint two-phase flow simulation in each iteration. Numerical results are presented which show that our technique is able to recover simultaneously in a stable and efficient way different regions and internal permeability profiles from two-phase flow data for realistic situations in 2D.

IC/MP176/155: Mathematical challenges in medical and industrial imaging, I and II.

Organiser: Richard Kowar (Universität Innsbruck, Austria)
Co-organiser: Markus Haltmeier (Universität Innsbruck, Austria)

Computer aided non-invasive medical imaging and non-destructive industrial testing of materials can be improved by either enhancing currently available data or by developing new imaging modalities. In these two minisymposia we present both, novel modalities and novel mathematical algorithms. We cover the three main aspects of imaging, namely data acquisition, modeling and reconstruction theory. However, our minisymposia will focus on mathematical reconstruction theory, which is often the key for improving imaging quality and the success of a special application in industry and medicine.

The first minisymposium presents various applications of mathematical image reconstruction theory involving *wave phenomena* and exploiting *phase information*. It starts with a talk about the application of a new non-iterative fully three-dimensional imaging technique based on the *sampling* or *factorization method* to improve the quality of metal detectors. The second talk is about a direct inversion method for the wave equation, based on *time reversal*, with various applications such as thermoacoustic CT in heterogeneous media, underwater communication or lithotripsy (a medical technique to destroy kidney stones). The last two talks are concerned with the modeling, data acquisition and with novel imaging reconstruction methods in *phase contrast microscopy* and *schlieren tomography*.

The second minisymposium is entirely devoted to *thermoacoustic computed tomography* (CT), also called photoacoustic or optoacoustic CT. Thermoacoustic CT has the potential to become a major imaging method for non-invasive medical diagnosis. Its physical origin is the generation of acoustic waves by optical or thermal excitation. However, the key to its success is the development of proper reconstruction algorithms, involving the stable solution of problems of integral geometry (the theory of recovering of a function from its integrals over certain manifolds). The first talk in this minisymposium gives an overview over various modalities of data acquisition in thermoacoustic CT. In the remaining talks of the first minisymposium mathematical models and novel fast reconstruction algorithms are presented.

Sampling methods for low-frequency electromagnetic imaging. **Bastian Gebauer** (RICAM Linz, Austria), Martin Hanke (Universität Mainz, Germany), Christoph Schneider (Universität Mainz, Germany) IC/MT1653/155

We consider the problem of detecting objects by electromagnetic imaging; i.e., by applying time-harmonic surface currents on an electric device and measuring the backscattered electromagnetic field. Numerical studies show promising results for new non-iterative reconstruction techniques known as linear sampling methods. Using a low-frequency approach we give a theoretical justification for these methods and discuss the consequences of divergence-free conditions.

A direct method for the numerical time-reversal of waves in a heterogeneous medium. **Christian Clason** (TU München, Germany) IC/MT1769/155

We consider the problem of time reversal in a heterogeneous medium as the inverse problem of determining the solution of a wave equation with spatially varying coefficients from lateral Cauchy data. This problem occurs in several applications in the area of medical imaging and non-destructive testing.

Using the method of quasi-reversibility, the original ill-posed problem is replaced with a boundary value problem for a fourth order partial differential equation. We find a weak H^2 solution of this problem and show that it is a well-posed elliptic problem. Error estimates and convergence of the approximation follow from exact observability estimates for the wave equation, which are proven using a Carleman estimate. We derive a numerical scheme for the solution of the quasi-reversibility problem by a B-spline Galerkin method, for which we give error estimates.

Finally, we present numerical results supporting the robustness of this method for the reconstruction of the wave field from lateral Cauchy data, where we also consider the case of data given only on a part of the boundary.

Phase-contrast measurement techniques: some aspects about phase microscopy and Schlieren imaging. **Bettina Heise** (Universität Linz, Austria), Bernd Arminger (Universität Linz, Austria) IC/MT1667/155

Phase contrast microscopy (PCM), differential interference contrast microscopy (DIC) and Schlieren imaging belong to the traditional techniques for visualization of transparent objects which can be described by their phase map. The first two methods have found their usual application in cell biology, whereas Schlieren Imaging can be used in visualization of flows in fluid dynamic processes or of pressure fields. Although these methods possess high spatial resolution, the challenging task is to extract quantitative results from the images. For DIC imaging an approximation of the phase map can be obtained by deconvolution or by line integration methods using different shear directions. In quantitative phase microscopy (QPM) three differently focused images are recorded and the phase map can be calculated.
In contrast, the approach used in holographic interferometry is to record several images with defined phase shifts introduced e.g. by a piezoelectric transducer (PZT) or electro-optically by a spatial light modulator and to perform a trigonometric reconstruction to obtain quantitative values.

3D reconstruction of transducer pressure fields from Schlieren data. **Richard Kowar** (Universität Innsbruck, Austria) IC/MT1247/155

In order to ensure safety and optimal performance of medical ultrasound transducers it is necessary to measure the acoustic pressure fields of transducers. For the estimation of such pressure fields we use light intensity data that is obtained by a Schlierensystem. Schlieren data corresponds mathematically to squared x-ray tomographic data. Acoustic pressure fields attain positive and negative values, but only the square of the line integrals are provided by the Schlieren system. Therefore the signs of the line integrals are not known, and Schlieren data cannot be reduced to data of classical X–ray CT. For the numerical estimation of pressure fields we used the loping Landweber-Kaczmarz method.

IC/MP176/155: Mathematical challenges in medical and industrial imaging, I and II. #2

Organiser: Richard Kowar (Universität Innsbruck, Austria)
Co-organiser: Markus Haltmeier (Universität Innsbruck, Austria)

(For abstract, see session #1 above.)

Thermo-acoustic tomography: effects of ultrasound-pulse softening on reconstructed images. **Sarah Patch** (University of Wisconsin, Milwaukee, USA) IC/MT1327/155

Thermoacoustic computerized tomography (TCT) is a hybrid imaging technique exploiting the thermoacoustic effect. TCT has many parallels with xray CT, including frequency dependent attenuation of the measured signal. However, the nature of these attenuation phenomena is nearly opposite: xray beams Şharden,Ť whereas ultrasound pulses Şsoften.Ť Analytic formulae for a attenuated TCT pulses generated by a homogeneous spherical inclusion immersed in soft biological tissue and also in highly attenuating fluids are presented. Resulting artifacts in reconstructed xray CT and TCT images are compared and contrasted.

New reconstruction formulas and algorithms for problems of thermo-acoustic tomography. **Leonid Kunyansky** (University of Arizona, USA) IC/MT2546/155

The problem of image reconstruction in the thermoacioustic tomography is equivalent to the inversion of the spherical mean Radon transform. In other words, the unknown function is reconstructed from a family of its spherical integrals or means. The centers of integration spheres usually lie on a closed surface surrounding the object (the support of the sought function). Explicit inversion formulas are known for the case when this surface is a sphere. We present a series solution of the reconstruction problem, valid for several other surfaces of practical importance (such as, for example, surface of a cube or of a finite cylinder). For the case of the cubic measuring surface we also develop a fast reconstruction algorithm. The use of this technique accelerates the computation by a factor of several hundred and reduces reconstruction from hours to several seconds.

Comparison of different scanning geometries for photoacoustic tomography using line detectors. **Robert Nuster** (Universität Graz, Austria), Guenther Paltauf (TU Graz, Austria), Markus Haltmeier (Universität Innsbruck, Austria), Peter Burgholzer (Upper Austrian Research) IC/MT1849/155

Photoacoustic tomography is an emerging procedure for imaging of small biological samples. The combination of optical contrast and acoustical resolution of photoacoustic imaging is the advantage in comparison to pure optical and acoustical imaging.

The current method to realise photoacoustic tomography is to use arrays of ultrasound transducers or single detectors scanning around the object to record the acoustic signals excited by illumination of the sample with short laser pulses. An important factor limiting the image resolution is the finite size of the detectors. In an effort to partly overcome this limitation we propose to use detectors that are larger than the object and integrate the incoming acoustic wave over their volume. This approach requires special reconstruction algorithms. If the detector is a plane scanning around the object the recorded set of acoustic signals corresponds to the three-dimensional Radon transform of the initial pressure distribution in the object. In this case an image can be reconstructed with the standard inverse Radon transform.

In this study we investigate signal collection procedures and image reconstruction algorithms that are designed for detectors having the shape of a line with a length exceeding the size of the object. Recent experiments, using a scan of the line shaped detector only in one direction, show that the image is blurred in this direction. This undesirable effect can be limited by using two scanning directions perpendicular to each other to record the missing data. The resolution of the image is only limited by the width of the line and the temporal resolution of the detector.

Limited-angle inversion of the circular Radon transform. **Markus Haltmeier** (Universität Innsbruck, Austria) IC/MT2761/155

In this talk we study the recovering of a function from its circular Radon transform, or equivaently from its integrals over circles. This is the main problem that arises in photo-/thermoacoustic tomography with integrating line detectors. Recently exact inversion formulas have been found for full angle data where the center set is a circle enclosing the unknown function. However, in many practical applications, such as in breast cancer detection with photo-/thermoacoustic tomography, the center set does not enclose the unknown function. Theoretically, certain features of the object can be recovered stably. However, no stable direct algorithm for inverting such data is known. In this talk we compare iterative methods with data continuation methods for limited-angle inversion.

IC/MP75/155: Variational methods for real-world problems.

Organiser: Abul Hasan Siddiqi (King Fahd University, Saudi Arabia)
Co-organiser: Martin Brokate (TU München, Germany)
Co-organiser: Pammy Manchanda (Guru Nanak Dev University, India)

Variational methods have played a vital role in understanding properly various real world problems. Variational inequalities and inverse problems are two themes which have attracted attention of a large number of researchers in different disciplines. The main objective of the minisymposium is to discuss certain current trends concerning variational inequalities and inverse problems.

Models for plasticity with variably-shaped yield surfaces. **Martin Brokate** (TU München, Germany) IC/MT3493/155

Standard constitutive models in plasticity like isotropic or kinematic hardening involve yield surfaces which are not constant in stress space, but their degrees of freedom are either translation or enlargement. In this talk we discuss mathematical results which apply also to yield surfaces which, in dependence on the loading history, change their shape in a rather general manner.

On relaxed viscosity iterative methods for variational inequalities in Banach spaces. **Qamrul Hasan Ansari** (King Fahd University, Saudi Arabia), Lu-Chuan Ceng (Shanghai Normal University, PR China), Jen-Chih Yao (National Sun Yat-sen University, Taiwan) IC/MT1644/155

Let $\tilde{J}$ be a commutative family of non-expansive self-mappings on a nonempty closed convex subset C of a reflexive Banach space X such that the set of common fixed points is nonempty. In this paper, we suggest and analyze a relaxed viscosity iterative method for a commutative family of nonexpansive self-mappings on C. We also prove that the sequence of approximate solutions generated by the proposed method converges strongly to a solution of a variational inequality. Our relaxed viscosity iterative method is the extension and variant form of the original viscosity iterative method. Results proved in this paper may be viewed as an improvement and generalization of the previously known results in the literature.

Fitting TAR(1)-models to Shepard data. **Torsten Lindström** (University of Kalmar, Sweden) IC/MT3862/155

This paper addresses some problems regarding two approaches commonly used in population dynamics. The first one is the mechanistic approach starting from assumed mechanisms (Metz and Diekmann, 1986). It formulates models based on these mechanisms and makes predictions regarding the long-run population dynamics predicted when these mechanisms really govern the dynamics. The other approach starts from collected data and aims at the best possible short term dynamics usually by training the model to predict the patterns present in the data. Such methods (Hastie and Tibshirani, 1990) usually penalize nonlinearities in the models fitted to the data and if the correct model is nonlinear, also the correct model is penalized.

In the former approach bounded populations usually mean nonlinear models meaning that we are in a situation where we do not expect that these methods confirm each other unless large amounts of data are available. This is usually not the case in population dynamics. The former approach has the advantage over the second that it has the potential to predict dynamical patterns not present in the data. The problem is that the mechanisms assumed are never confirmed to be the governing ones unless the two approaches can be matched and we shall deal with theoretical problems arising when matching those two approaches.

We demonstrate the following results:

(1) We recall the bifurcation diagram of non-negative Schwartzian derivative maps used for the study of population cycles in Stenseth, Chan, Framstad, and Tong (1998) and Lindström and Thunberg (2006).
(2) A nonlinear Sheperd (1982) model is used for generating nonlinear data and the above models are fitted to these data. We show that the dynamics of the fitted models do not in general conform with the dynamical patterns of the Sheperd (1982) models.
(3) We also fit the nonlinear Ricker (1954) model to the same data showing that fitting a false nonlinear model to the given data produce even worse correspondences between original dynamics and fitted dynamics than in the former case. Nonlinear data-fitting can thus, not remedy the problems reported here even if they in principle would have the potential to follow the dynamics of the original model quite precisely.
(4) Finally, we fit Multivariate Adaptive Regression Spline (MARS)-models (Friedman, 1991) models having possibilities to recover most periods and dynamical patterns in the original data but detect switching phenomena already at low periods and low noise level. In these switching windows, the Sheperd model may display periodic behaviour whereas the fitted MARS-model displays non-periodic behaviour.

One additional problem is we do not have any information regarding the uniqueness of the periodic attractors of the MARS models. Such results exist for TAR(1)-models (Lindström and Thunberg, 2006).

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IC/MP75/155: Variational methods for real-world problems. #2

Organiser: Abul Hasan Siddiqi (King Fahd University, Saudi Arabia)
Co-organiser: Martin Brokate (TU München, Germany)
Co-organiser: Pammy Manchanda (Guru Nanak Dev University, India)

(For abstract, see session #1 above.)

On the uniform decay in an integro-differential elastic equation. **Messaoudi Salim** (King Fahd University, Saudi Arabia) IC/MT2877/155

In this work, we consider a second-order problem:

$$\begin{cases} u_{tt} - \sum_{i,j=1}^{n} \frac{\partial}{\partial x_j}(a_{ij}(x)\frac{\partial u}{\partial x_i}) + \int_0^t g(t-\tau)\sum_{i,j=1}^{n} \frac{\partial}{\partial x_j}(a_{ij}(x)\frac{\partial u}{\partial x_i})(\tau)d\tau = 0, & \text{holds within } \Omega\times(0,\infty) \\ u(x,t) = 0, & \text{for } x \in \partial\Omega,\ t \geq 0 \\ u(x,0) = u_0(x), u_t(x,0) = u_1(x), & \text{for } x \in \Omega \end{cases}$$

This type of problem models the deformation in an elastic material of memory type.

Under suitable conditions on g, we establish a uniform decay. Precisely, we show that the decay is exponential if g decays exponentially and the decay is polynomial if g decays in a polynomial fashion. This work generalizes the decay result, proved earlier for wave equations with integral term, to the above problem.

Analysis of the relationship between the ENSO and sea-level changes. **Zafer Aslan** (Istanbul Aydın University, Turkey), Z. Can (Istanbul Aydın University, Turkey), O. Oguz (Istanbul Aydın University, Turkey) IC/MT5039/155

The relationship between ENSO with ONI and sea-level (SL) changes are analyzed to define the role of ELNINO3.4 on sea level variations around Turkey and Indian coasts by using monthly sea level time series at 25 sites. There are positive correlation between SL and ENSO and ONI (warm and cold episodes) based on a threshold of +/- 0.5°C for the Oceanic Niño Index (ONI) based on the 1971–2000 base period. For historical purposes cold and warm episodes are defined when the threshold is met for a minimum of 5 consecutive over-lapping seasons. Different techniques have been used to define El Niño event. The most common ones are the Southern Oscillation Index (SOI) and the Niño regions. The Niño regions refer the SST anomalies in defined parts of the Tropical Pacific. There is sufficient evidence on the relation between time series analysis of Sea Level values and ELNINO indices. In northern coastal part of Turkey, the role of positive effect is high. At the western coastal part of Turkey the relation between ELNINO indices and SL is negative. This relation can also be interpreted by applying 1-D wavelet and continuous wavelet packets on data. Cross-correlation maps at regional scale for Turkey and India have been presented.

High-index differential-algebraic equations and application to trajectory optimization. **Soumyendu Raha** (Indian Institute of Science Bangalore) IC/MT924/155

Trajectory optimization problems arise in robotics and design of nominal guidance and control for aero-space vehicles. The present study is in the context of re-entry to landing trajectory optimization of reusable space vehicles. The trajectory problem is a high index differential-algebraic equations (DAE) model resulting from rigid body dynamics of the vehicle constrained by heat flux, loading and landing speed requirements. This kind of DAE models are common for many other areas of engineering and the computational and numerical methods studied can be extended to those problems without loss of generality. The present study develops a damped discretization for the method of transcription solution to the problem. The effect of damping has been studied in the context of convergence and stability of the iterates generated by the transcription method in a sequential quadratic programming (SQP) like non-linear programming (NLP) solver. This computational study has been contrasted with index reduction approaches. Numerical examples are given to illustrate the results.

Existence and iterative approximation of solutions of some systems of variational-like inequalities and inclusions. **Syed Khan** (Aligarh Muslim University, India), Kaleem Kazmi (Aligarh Muslim University, India) IC/MT2864/155

Variational inequality theory introduced by Stampacchia and Fichera independently, in early sixties in potential theory and mechanics, respectively, constitutes a significant extension of variational principles. The development of variational inequality theory can be viewed as the simultaneous pursuit of two different lines of research. On the one hand, it reveals the fundamental facts on the qualitative behavior of solutions to important classes of problems. On the other hands, it enables us to develop highly efficient and powerful numerical methods to solve, for example, obstacle, unilateral, free and moving boundary value problems. One of the most important and interesting problem in the theory of variational inequalities is the development of numerical methods which provide an efficient and implementable algorithm for solving variational inequalities and its generalizations. Some of such methods are projection methods and its various forms; proximal-point mapping method, linear approximation, descent and Newton's methods, and the methods based on auxiliary principle technique. In 1985, Pang [Math. Prog. **31** (1985) 206-219] showed that a variety of equilibrium models, for example, the traffic equilibrium problem, the spatial equilibrium problem, the Nash equilibrium problem and the general equilibrium programming problem can be uniformly modelled as a variational inequality defined on the product sets. He decomposed the original variational inequality into a system of variational inequalities and discuss the convergence of method of decomposition for system of variational inequalities. Later, it was noticed that variational inequality over product sets and the system of variational inequalities both are equivalent. Since then many authors studied the existence theory of various classes of system of variational inequalities by exploiting fixed-point theorems and minimax theorems. On the other hand, only a few iterative algorithms have been constructed for approximating the solution of system of variational inequalities.We remark that most of the work on approximate solvability of variational (-like) inclusions and systems of variational (-like) inequalities has been done in the setting of *Hilbert spaces*.
vspace.20cm

Motivated by the recent research work in this directions, we consider some systems of variational (-like) inequalities and inclusions; develop the iterative algorithms for finding the approximate solutions and discuss their convergence criteria. Further, we study the sensitivity analysis of solution of the system of variational inclusions. The techniques and results presented here improve the corresponding techniques and results for the variational inequalities and inclusions in the literature.

System of variational inclusions Let, for $i = 1,2$, E_i is q_i-uniformly smooth Banach space with norm $\|.\|_i$.Let $g_i, A_i, B_i : E_i \to E_i$ be nonlinear mappings; let $F : E_1 \times E_2 \to E_1, G : E_1 \times E_2 \to E_2$ be two nonlinear mappings, and let $M : E_1 \to 2^{E_1}$, $N : E_2 \to 2^{E_2}$ be m_i-accretive, respectively, such that $g_i(x) \in domainM_i(.)$, for all $x \in E_i$. We consider the following system of general variational inclusions (SGVI): Find $(x,y) \in E_1 \times E_2$ such that

$$\begin{cases} F(A_1(x), A_2(y)) + M(g_1(x)) \ni \theta_1; \\ G(B_1(x), B_2(y)) + N(g_2(y)) \ni \theta_2, \end{cases} \tag{4.1}$$

where θ_1 and θ_2 are zero vectors of E_1 and E_2 respectively.Using proximal-point mapping technique, we prove the existence and uniqueness of solution and suggest a Mann type perturbed iterative algorithm for SVLI. Furthermore, we discuss the convergence criteria and stability of Mann type perturbed iterative algorithm. Further, we consider a system of parametric general variational inclusions (in short SPGVI) corresponding to SGVI and discuss the continuity of the solution.

System of variational-like inequalities Let $I = \{1,2\}$ be an index set and for each $i \in I$, let H_i be a real Hilbert space whose inner product and norm are denoted by $\langle .,. \rangle_i$ and $||.||_i$, respectively. For each $i \in I$, let $F_i : H_1 \times H_2 \to H_i$, $\eta_i : H_i \times H_i \to H_i$, $g_i : H_i \to A_i$, $g_i : H_i \to H_i$, $B_i : H_i \to H_i$ be nonlinear mappings, then we consider the following system of generalized variational-like inequality problems (SGVLIP):

Find $(x,y) \in H_1 \times H_2$ such that

$$\langle F_1(A_1(x), A_2(y)), \eta_1(g_1(v_1), g_1(x)) \rangle_1 + b_1(x, g_1(v_1)) - b_1(x, g_1(x)) \geq 0, \ \forall v_1 \in \tag{2.1}$$

$$\langle F_2(B_1(x), B_2(y)), \eta_2(g_2(v_2), g_2(y)) \rangle_2 + b_2(y, g_2(v_2)) - b_2(y, g_2(y)) \geq 0, \ \forall v_2 \in \tag{2.2}$$

where for each $i \in I$, the bifunction $b_i : H_i \times H_i \to R$, which is not necessarily differentiable, satisfies some suitable conditions. We prove an existence theorem for auxiliary problems of SGVLIP. Further, by exploiting this theorem, an algorithm for the SGVLIP is constructed. Furthermore, we prove the existence of a unique solution of SGVLIP and discuss the convergence analysis of the algorithm. **Remark:**

(i) Using the approaches given here, one can extend Theorems presented here to the systems of n-variational-like inclusions and inequalities.
(ii) It is of further research interest to extend the approaches discussed in this talk for iterative approximation of solutions of the systems of variational-like inclusions and inequalities, involving set-valued mappings.

IC/MP654/155: Inverse problems and applications II: soft-field tomography in engineering.

Organiser: Manuchehr Soleimani (University of Manchester, UK)
Co-organiser: Oliver Dorn (Universidad Carlos III de Madrid, Spain)

Mathematical techniques play a growing role in many engineering applications. Often novel mathematical concepts are needed in order to meet the rapidly evolving requirements of the practitioners. One prominent example of such a research area is soft-field tomography. In the session, four experts will present examples of such novel mathematical techniques emerging in this exciting research area. Examples are atomic force spectroscopy, tomographic image reconstruction and dynamic process tomography.

Force spectroscopy in atomic-force microscopy. **Nick Polydorides** (University of Cyprus) IC/MT1358/0

This work is motivated by the inverse force spectroscopy problem in atomic force microscopy. In the formulation of the forward problem we consider the Euler-Bernoulli model for flexural vibration of an AFM cantilevered beam of finite length, under the influence of a distributed load force. Our aim is to show that the profile of the load force can be inferred by sampling the vertical displacement of the vibrating beam. Accounting for the appropriate boundary and initial conditions, we derive the GreenŠs function of the system and cast the solution of the problem in an integral equation form. In this context, we approach the inverse problem using *a priori* information about the plausible deformations of the cantilever beam.

Challenges in mathematics for electrical capacitance tomography. **Wuqiang Yang** (University of Manchester, UK) IC/MT1497/0

There are two major problems to be solved with electrical capacitance tomography (ECT): the forward problem and the inverse problem. Because ECT is based on soft field sensing and the relationship between capacitance and permittivity is non-linear, it is difficult to solve the forward problem analytically. While a finite element method (FEM) or finite difference method (FDM) may be used, depending on the geometry of a sensor, to solve the forward problem numerically, a major challenge remains to find a solution accurately and quickly. Usually, the number of capacitance measurements in a data set is much less than the number of pixels in an image. Obviously, the solution to the inverse problem is under-determined. Furthermore, the inverse matrix is ill-posed and ill-conditioned. This presents a major challenge in mathematics. This paper will discuss the above challenges. Some image reconstruction algorithms will be discussed in detail, such as the relaxation factor, semi-convergence and the convergence speed. While iterative algorithms are considered by mathematicians and feedback control by control engineers independently, it seems that the concept and terminology used in the two fields are corresponding to each other. It would be interesting to see how control system design can benefit iterative image reconstruction. As 3D ECT is being investigated at several research institutions, this paper will discuss some specific challenges with 3D ECT, including measurement strategy, a finite volume method (FVM), the condition number of sensitivity matrix, and demanding on computation and memory.

Adaptive importance sampling in particle filter based dynamic process tomography . **Daniel Watzenig** (TU Graz, Austria), Gerald Steiner (TU Graz, Austria), Markus Brandner (TU Graz, Austria) IC/MT1737/0

The estimation of cross-sectional material distributions from non-stationary sparse tomographic measurement data is a demanding class of ill-posed inverse problems. Electrical Capacitance Tomography (ECT) is a well-established modality that aims at monitoring and controlling dynamic industrial processes arising e.g. in pneumatic conveying or heterogeneous flow fields. Due to its low cost, good dynamic behavior and operability under harsh environmental conditions, ECT has gained importance over the last decade. By measuring the capacitances between certain electrodes that are arranged around the periphery, the permittivity distribution inside closed objects can be spatially resolved.

In this paper, the main focus is on the robust estimation of time-dependent process metrics like void fraction and fill level given uncertain measurements. The underlying inverse problem is formulated in a Bayesian inferential framework, by accurately modeling the forward map, specifying a prior distribution for the cross-sectional material distribution, and characterizing the statistics of the measurement noise, to give a

posterior distribution for relevant process parameters conditioned on measured data. The forward map is numerically implemented using the Finite Element Method (FEM). Transitions between different material phases are described by means of a Fourier contour model of second order implying a geometric regularization yielding smooth shapes in the image space. Sequential Monte Carlo filtering – particle filtering – is applied to solve the non-stationary inverse ECT problem. Consequently, the inverse ECT problem is recast as a state estimation problem. In order to improve the filter performance adaptive importance sampling based on the residual error information is proposed. This modification of the filter algorithm allows for fast detection of time-varying material inclusions that may appear in different regions of the cross-sectional area of pipes. Based on a significant change in the residual error, particles are scattered in regions where the inter-electrode capacitances have changed indicating a variation of the electric properties in that area. Furthermore, the issue of recognizing an empty pipe is addressed by monitoring the error variance of the all particles. The posterior variability of estimated process metrics is evaluated to give statements on the parameter confidence. Different experiments are performed in order to show the robustness of the Bayesian filtering approach to solve the non-stationary inverse problem given measured electrical capacitance data.

Subspace-based reconstruction algorithms for the inverse problem of electrical impedance tomography. **Ronny Hoffmann** (Vrije Universiteit Brussels, Belgium), Bart Truyen (Vrije Universiteit Brussels, Belgium), Jan Cornelis (Vrije Universiteit Brussels, Belgium) IC/MT1941/0

We present a subspace based, structure preserving solution method for the problem of Electrical Impedance Tomography, where the conductivity inside a simply connected 2-dimensional domain is sought from noisy and incomplete boundary data. Unlike conventional output-least squares algorithms that can be regarded as minimizing a certain error norm, solutions are recovered here as the minimizers of a closely related residual norm problem. An iterative solution scheme is shown to lead to a sequence of sparse matrix subproblems, with conditioning far more favorable than typically observed in output-least squares. We find that these sparse subproblems demonstrate a particular form of displacement structure that can be further elaborated to finally arrive upon an efficient computational implementation. In this contribution we introduce the structured problem formulation, outline the algorithmic approach taken, and summarize some of its numerical properties.

IC/MP1076/015: Optimal control of industrial applications modelled by DAEs and P(D)AEs.

Organiser: Kurt Chudej (Universität Bayreuth, Germany)
Co-organiser: Matthias Gerdts (University of Birmingham, UK)

Optimization and optimal control of huge realistic models of industrial applications are challenges for applied mathematiciens. Although the applications come from different fields like container cranes, cars and power plants, the mathematical problems are very similiar. New tailored approaches and generalized theory are necessary to cope with the huge complexities of the models.

Optimal control, simulation and model reduction of large PDAE-systems. **Armin Rund** (Universität Bayreuth, Germany), Hans Josef Pesch (Universität Bayreuth, Germany), Kurt Chudej (Universität Bayreuth, Germany) IC/MT2331/159

Molten carbonate fuel cells (MCFC) are especially well suited for stationary power plants if their process heat is used to increase their efficiency. MCFCs will become soon competitive compared with traditional power plants.

The dynamic behaviour of MCFCs can be modelled mathematically by a hierarchy of systems of partial differential algebraic equations (PDAE) in 1D or 2D. Integral terms appear and the nonlinear boundary conditions are given partly by a DAE system.

These large PDAE systems of dimension between roughly 10 and 30 equations are discretized by the method of lines, yielding huge dimensional DAEs. In order to enable real time control of the system model reduction techniques are needed. We will present new computationally expensive numerical results of (sub)optimal control during load changes for a 2D dynamical MCFC model.

Optimal control of an industrial robot by a non-smooth Newton's method. **Martin Kunkel** (Universität Hamburg, Germany) IC/MT2156/159

We investigate a nonsmooth Newton's method for the numerical solution of discretized optimal control problems subject to pure state constraints and mixed control-state constraints. The infinite dimensional problem is discretized by application of a general one-step method to the differential equation. By use of the Fischer-Burmeister function the first order necessary conditions for the discretized problem are transformed into an equivalent nonlinear and nonsmooth equation. This nonlinear and nonsmooth equation is solved by a globally convergent nonsmooth Newton's method. Numerical examples for the optimal control of a robot conclude the article.

Switching-times optimization for bang–bang and singular controls in bioprocess engineering. **Georg Vossen** (Universität Bremen, Germany) IC/MT2393/159

We will study optimal control problems with the control variable appearing linearly. The optimal control function in such problems often contains both bang-bang and singular arcs, i.e., it takes values at the boundary, resp., inside the control domain. These control problems occur in many industrial application fields such as mechanics, biotechnologies and medical sciences. A method of transforming the problem into a finite-dimensional optimization problem will be presented. This so-called induced optimization problem involves the (finitely many) switching times, all free initial state values and the free final time. On the one hand, this method is a strong tool for solving high-dimensional optimal control problems. On the other hand, one is able to check second-order sufficient conditions (SSC) for this problem in a numerically efficient way. Additionally, it is often interesting to investigate the influence of certain pertubations into the system. This parameter sensitivity can also easily be computed in the induced problem. We will show that the SSC test and the sensitivity analysis can be applied on the basis of only first order variations of the state trajectory which can be derived by solving simple linear initial value problems. All results will be illustrated with a model of the optimal control of a fed-batch fermentation process.

Optimal control of constrained time lag systems: necessary conditions and numerical treatment. **Laurenz Göllmann** (Westfälische Wilhelms-Universität Münster, Germany), Helmut Maurer (Universität Münster, Germany), Daniela Kern (Weierstraß-Institut Berlin, Germany) IC/MT3277/159

In this talk we consider retarded optimal control problems with constant delays in state and control variables under mixed control-state inequality constraints.

First order necessary optimality conditions in the form of Pontryagin's minimum principle are presented and discussed as well as numerical methods based upon discretization techniques and nonlinear programming. The minimum principle for the considered problem class leads to a boundary value problem which is retarded in the state dynamics and advanced in the costate dynamics.

It is shown that the Lagrange multipliers associated with the programming problem provide a consistent discretization of the advanced adjoint equation for the delayed control problem.

Finally, the theory and the proposed numerical method are illustrated by an example from chemical engineering. We discuss the optimal control of a continuous stirred chemical tank reactor system (CSTR) in order to apply the proposed algorithm and to compare the computed results with the theory. Due to significant transportation times given by the flow rate of the chemical reactants some state and control variables enter the dynamic equations of the CSTR with a delay.

15: Modelling and Simulation, Contributed Talks

IC/CTS4648/15: **Numerical methods for industrial applications.**

Organiser: Vedpal Singh (IIT Roorkee, India)

Analyzing securitization processes using simulation methods. **Marcin Wierzbicki** (Military University of Technology, Poland), Radoslaw Pytlak (Military University of Technology, Poland) IC/CT2862/015

The aim of this paper is to describe the securitization process and factors which affect it. At the beginning we present shortly the purpose and key elements of securitization, from creating a mortgage pool to issuing CMO certificates and passing mortgage payments to certificate holders. Then we pinpoint two main elements, namely interest rate models and prepayment models, and show their impact on securitization of a mortgage pool. First we consider interest rate models. We compare briefly different interest rate models including classical short rate models, HJM class models and the String Market Model presented by Santa-Clara and Sornette,

$$d_t f(t,x) = \alpha(t,x)dt + \sigma(t,x)d_t Z(t,x), \qquad (1)$$

We present the descritized version of (1) which does not allow the arbitrage. We also show two calibration approaches: historical and market prices. After that, we mention few prepayment models and pay special attention to optimal recursive refinancing shown by Longstaff which uses regression and dynamical programming techniques. At the end, we combine all elements to define an optimization problem that can be used to increase the efficiency of securitization problems. We define the efficiency in two ways. The first one is to maximize CMO issuer profits. We can define profits as a function of four cash flows: payments made to the crediting bank, payments made by CMO certificate holders, mortgage scheduled payments, and CMO certificates scheduled payments. The second way is to propose a securitization scheme under the assumption that Z-tranche is unattractive to investors. We illustrate that 'ad hoc' securitization may be far less efficient than solving an optimization problem.

A mathematical model for longevity prediction of lacquer-paint coatings in sea water. **Victor Shevchuk** (National Academy of Sciences of Ukraine, Kyiv), Pavlo Shevchuk (Pidstryhach Institute, Ukraine) IC/CT563/010

The prediction of longevity of lacquer-paint protective coatings in aggressive environments is an important problem, which is usually solved on the basis of long-term and expensive testing. However, it is possible to elaborate an adequate mathematical model of coatings aging for analytical calculations of coating lifetime, using geometrical and physicomechanical parameters of the model experimentally determined in laboratory conditions. Since the mechanism of coatings destruction during exploitation in sea water is extremely complicated and includes a great number of consecutive and parallel physico-chemical and structural changes, the development of the mathematical model of such a complicated mechanism needs its formalization. This formalization takes into account the main processes of the mechanism and provides the possibility of its mathematical description.

This paper presents a polyparameter mathematical model, which has been elaborated with the use of the methods of continuum mechanics and non-equilibrium thermodynamics. The model is based on the detailed study of the laws of physico-chemical, electrochemical and other processes in the system sea water-coating-metal base, on the analysis of the failure mechanism of coatings and on certain results of purposeful laboratory measurements.

To simplify the model, the whole process of coating aging in sea water is represented in the form of a number of subsequent stages with the mathematical description of determining physical parameters on each of them up to cohesive or adhesive failure of a coating. For each of these typical stages of the coatings aging process, the appropriate linear or nonlinear boundary value problems of mathematical physics have been formulated, and the procedure of their analytico-numerical solving has been elaborated.

The numerical investigations allow discovering a number of the new regularities of coatings aging. The elaborated mathematical model gives possibility to predict the lifetime of coatings, to quickly analyze the influence of their certain characteristics, operation conditions, and technological factors on the coatings longevity, to optimize the parameters of newly constructed coatings with the aim of increasing their durability and to make appropriate corrections still on the stage of their production.

The application of the FDEM program package with error estimate to industrial problems. **Torsten Adolph** (Forschungszentrum Karlsruhe, Germany), Willi Schönauer (Forschungszentrum Karlsruhe, Germany) IC/CT2245/015

The Finite Difference Element Method (FDEM) program package is a robust and efficient black-box solver that solves arbitrary non-linear systems of elliptic and parabolic partial differential equations under arbitrary non-linear boundary conditions on arbitrary domains in 2-D and 3-D. FDEM is an unprecedented generalization of the finite difference method on unstructured finite element meshes. From the difference of formulas of different order we get an easy access to the discretization error. By the knowledge of this error the mesh may be refined locally to reduce the error to a prescribed relative tolerance. The error estimate is a unique property for such a general black-box. In addition, the FDEM program package is efficiently parallelized on distributed memory parallel computers.

In this paper we demonstrate the usefulness of the FDEM program package by its application to several industrial problems. This gives completely new results as up to now people have solved these problems blindly, unaware of the error of their solution.

The first problem is the numerical simulation of a microreactor where we have two chemical components entering through the main channel and two chemical components entering through a side channel so that there is a reaction of two of the components. We want to examine the flow field and the behaviour of the chemical components.

The second problem is the simulation of the distribution (and possibly of the combustion) of hydrogen in an open domain. We have a small opening at the bottom where the hydrogen enters into the domain filled with air at the beginning.

Thirdly we simulate numerically a high-pressure discharge lamp where we have a constant plasma arc between two electrodes.

Finally we simulate the distribution of the temperature in a DC/AC-converter module with 6 power-MOSFETs heated with uniform power. At the bottom of the module air cooling is applied. In contrast to the first 3 elliptic problems this is a 3-D parabolic problem.

The optimal spatial deployment of radiation portal monitors to improve nuclear detection at overseas ports. **Yifan Liu** (George Mason University, USA) IC/CT2847/158

Radiation portal monitors are starting to be deployed at overseas ports to prevent nuclear weapons from entering the U.S. in a shipping container. Current designs have containers on trucks passing through a portal monitor at approximately 10 mph, before being routed to one of several lanes at the port's front gate for a driver identification check. For a fixed cost of testing, which consists of the costs of radiation portal monitors plus offsite x-ray and possibly manual testing of containers generating a false radiation alarm that cannot be resolved by gamma-ray imaging, we compare the neutron detection limits of the current design and three other designs that do not affect truck congestion at the front gate. Putting a portal monitor at the head of a single queue before trucks are routed to a lane reduces the detection limit by a factor of 2 over the current design. Placing one monitor in each lane, so that testing occurs during processing, improves the detection limit by an additional factor of 4, and using N additional monitors in n sets, each set within the length of a container, requires optimization algorithms to find the best n. Using a mile-long corridor of monitors in tandem could reduce the detection limit by several more orders of magnitude, thereby allowing the detection of highly-enriched uranium.

Integer solution of a set of bilinear equations. **Mariusz Ziolko** (AGH University of Science and Technology, Krakow„ Poland), Michal Nowak (Akademia Górniczo-Hutnicza, Poland) IC/CT1057/015

Transmultiplexer combines several digital signals into a single one. At the transmitter side the M input signals are upsampled, filtered and summed to obtain a composite signal. This signal is sent through a single transmission channel to all recipients. At the receiver side, the composite signal is split into M channels for separation. The signal is filtered and downsampled to obtain the output signals. This system contains linear and time-invariant elements. This facilitates mathematical modelling. The basic idea is the reversibility of all procedures in such a way that all signals could be recovered as precisely as possible. A transmultiplexer achieves perfect reconstruction if output signals are only a delayed version of input signals. To design a transmultiplexer system means to determine such coefficients that fulfil some algebraic equations. This is a difficult task due to the fact that equations are bilinear. One can use numerical procedures to determine filter coefficients by minimizing the residua obtained from equations. Sometimes it is possible to obtain solutions for simple systems. In general however, there are no known methods to solve a set of bilinear equations. What is more, it is difficult even to examine the existence and uniqueness of solutions. Looking for solutions leads to determining the sufficient conditions that can be written in a more simple form. A procedure of this kind will be presented in our paper. Computational algorithm resulting from the theorem and a simple example will be presented as well. Till now, the perfect reconstruction conditions are fulfilled only theoretically because the quantization errors in digital filtering for real numbers are inevitable. Practically, output signals were a little different than input ones. Our method enables to provide all calculations using integer numbers only. Due to the incorporation of integer values, a perfect reconstruction can be realized not only theoretically but also in practice. Thanks to that, transmultiplexer systems equipped with integer filters can be used not only to transmit multimedia signals but also for encrypted data, lossless compressed signals or for computer software data where a change in even one single bit is inadmissible.

Mathematical model for waste minimization of a bleach plant in the paper industry. **Vedpal Singh** (IIT Roorkee, India), Vivek Kumar (IIT Roorkee, India), Deepak Kumar (Indian Institute of Technology Roorkee,Saharanpur) IC/CT4787/159

Mathematical Model for Waste Minimization of a Bleach Plant in Paper Industry

V.P.Singh , Vivek Kumar , Deepak Kumar

Indian Institute of Technology Roorkee,Deptt. of Paper Technology,Saharanpur Campus,Saharanpur -247001, India Email: sighvp2@yahoo.co.on , Fax: +91-132-2714011.

ABSTRACT

Modern pulp bleaching appears to favour multistage bleaching sequences for the production of high brightness market pulp of good quality at low cost. The exact choice of bleaching sequence depends upon the type of pulp to be bleached and the level of the brightness to be achieved. A number of simulation studies have been carried out in order to minimize the amount of effluents from the bleaching plant. Myers et al. (1989, Tappi J. 72, 131-135) used GEMS for the optimum design and for the determination of operating conditions of an oxygen delignification system in order to minimize the delignification costs and to reduce the total organic chlorine emissions from the bleach plant. Brooks et al. (1994, Tappi J. 77, 83-92) used simulation to evaluate the conversion of a conventional oxygen delignified softwood bleach plant to TCF bleaching based on hydrogen peroxide. Parsad et al. (1996, Tappi J. 79, 144-152) made an economic analysis through simulation of a kraft-oxygen mill with modifications of the pre-bleaching and bleaching systems to incorporate TCF and closure issues.

In the present investigation a steady-state mathematical model is developed for a typical four stage CEHH bleaching sequence in Indian Pulp and Paper Industry.Each stage of the sequence is composed of chemical additions and mixing, reaction in a retention tower, and washing. Unit operation models were formulated using mass balances on liquor, fibres, kappa number, chemicals and COD based on the assumption of perfect mixing and quasi steady-state. The COD is used in this paper as an indication of the amount of effluent coming out from four bleaching stages. COD measurement of bleach plant effluent separately is not a routine mill measurement; so COD is calculated in the basis of correlation of COD given by Anjana (2001). In order to validate the model, the simulated results were compared the literature data ; a good agreement between the simulation results with the literature data is achieved. In the case studies, the optimization of the process variables are performed in which the effects of retention tower, operating temperature, residence time, consistency, bleaching liquor flow rate and the wash water flow rates in the washers are studied.

Keywords: Bleaching; Steady-state modeling ; CEHH; Process variable optimization; Waste minimization

IC/CTS4645/15: Analytical and numerical methods for heat conduction.

Organiser: Philippe Tanguy (École Polytechnique de Montréal, Canada)

Axisymmetric heat conduction in a multimaterial cylindrical solid. **Whye Teong Ang** (Nanyang Technological University, Singapore) IC/CT419/015

The axisymmetric steady-state heat conduction in a multimaterial cylindrical system is considered. The cylindrical system is made up of four possibly dissimilar materials occupying the regions R_1, R_2, R_3 and R_4 defined by $R_1 = \{(r,\theta,z) : r < r_2,\ 0 < \theta \le 2\pi,\ 0 < z < h_1\}$, $R_2 = \{(r,\theta,z) : r_1 < r < r_2,\ 0 < \theta \le 2\pi,\ h_1 < z < h_2\}$, $R_3 = \{(r,\theta,z) : r < r_1, 0 < \theta \le 2\pi, h_1 < z < h_2\}$ and $R_4 = \{(r,\theta,z) : r < r_2,\ 0 < \theta \le 2\pi,\ h_2 < z < h_3\}$, where r, θ and z are the cylindrical polar coordinates, and r_1, r_2, h_1, h_2 and h_3 are given real constants such that $0 < r_1 < r_2$ and $0 < h_1 < h_2 < h_3$. The interfaces between the materials are perfectly bonded. The curved part of the exterior boundary of the system, that is, the surface $r = r_2$, $0 < z < h_3$, is thermally insulated. Specific types of boundary conditions are imposed on the flat ends of the multimaterial cylinder, e.g. a uniform temperature may be prescribed on each of the flat ends. An analytical formula is derived for the temperature in the multimaterial solid. The coefficients of the truncated series are determined by solving a system of linear algebraic equations. The solution has practical applications in modern engineering, such as in thermal analysis of computer chips and carbon nanotubes. For example, R_1 and R_4 may represent two computer parts separated by a thermal interface material in R_2 whose thermal conductivity is enhanced by a carbon nanotube in R_3.

Numerical simulation of thermal hydraulics in an ADSS model. **BVRathish Kumar Bayya** (IIT Kanpur, India) IC/CT1250/015

Futuristic nuclear reactors like ADSS (Accelerator Driven Subcritical System) have evoked renewed interest in research because it operates in sub-critical conditions and transmutes radioactive nuclear wastes. In an ADSS, a high energy proton beam from the accelerator irradiates a heavy metal target to produce spallation neutrons, which initiate the fission reaction in the sub-critical core. The spallation target module is the most innovative component in the ADSS. The design of the spallation target module requires a fair understanding of the thermal-hydraulics involved, as a large amount of heat is generated in the system during the course of nuclear interactions with the molten liquid metal target. The window, a physical barrier separating the molten metal from the proton beam, is a critical component as it is subject to high heat fluxes, thermal and mechanical stresses. Even though it is relatively easy to take away the total spallation heat by the heavy metal target, what is crucial is that this has to be achieved without the the target temperature exceeding the stipulated temperature in any region of the flow. The presence of any recirculation or stagnation zones of fluid may lead to local hot spots either in the window or in the flowing liquid metal which is detrimental to the performance of the target. This necessitates detailed flow and heat transfer analysis in the spallation region, flow region near the entrance of the annular zone along with the temperature distribution of the window.

indent Numerical simulation has been accomplished using SUPG-FE method of Brooks and Hughes. The solution technique is based on the Eulerian velocity correction approach. This is essentially a variant of the projection scheme of Chorin , which was originally developed in a finite difference context and identical to the Marker And Cell (MAC) method. The computational grid was generated using algebraic method subsequently smoothened and clustered by elliptic partial differential technique using Poisson equation. Simulations have been carried out for various values of Reynolds numbers in laminar and turbulent regime to analyze the flow and temperature field.

indent A conjugate heat transfer analysis is accomplished to incorporate the physical operating situation of an ADSS in a more realistic way. The conduction equation of the beam window is solved in conjunction with the energy equation using the paradigm of domain decomposition parallelization method and the temperature distribution along the beam window is found. Finally, the thermal stresses and mechanical stresses along the radial and circumferential direction on the beam window is determined using temperature and pressure values. The radial stress values are higher compared to the circumferential stress for the case of mechanical stresses but vice versa in the case of thermal stresses.

Electromagnetic and thermal modelling of axisymmetric induction furnaces. **Maria del Carmen Muniz** (Departamento de Matemática Aplicada. Universidade, Spain), Alfredo Bermudez de Castro (Universidade de Santiago de Compostela, Spain), Dolores Gomez Pedreira (Universidade de Santiago de Compostela, Spain), Pilar Salgado (Universidade de Santiago de Compostela, Spain) IC/CT3834/010

A numerical method to describe the thermo-electric behavior of an induction heating furnace is introduced. It is obtained by using an enthalpy formulation concerning the thermal model and an integral representation of the electromagnetic potential in an unbounded domain. A BEM-FEM method is used and an iterative algorithm together with numerical results for an industrial heating system are presented.

A heat engine based on evaporative cooling at reduced pressure. **Noel Barton** (Sunoba Energy Systems, Australia) IC/CT1383/015

A thermodynamic model is presented for a heat engine based on evaporative cooling of hot dry air at reduced pressure. The principle of the new engine is the antithesis of conventional gas or vapour engines, which rely on heating at increased pressure. The new thermodynamic cycle is analysed for a two-stroke reciprocating piston version. The analysis includes the effect of water vapour in the air and further evaporation during re-compression. The engine will be bulky, but well suited to power generation from passive solar pre-heating. As a typical result, air at 35°C and 35% relative humidity pre-heated to 75°C can theoretically produce 3.7 kJ per kg dry air. That corresponds to efficiency of conversion of pre-heating to power of 8.4%. Even without pre-heating, evaporative coolers can produce power.

A fast and robust fictitious-domain method for modeling propellant flow in a three-blade planetary mixer. **Philippe Tanguy** (École Polytechnique de Montréal, Canada), Benjamin Coesnon (École Polytechnique de Montréal, Canada), Vincent Stobiac (École Polytechnique de Montréal, Canada), Francois Bertrand (École Polytechnique de Montréal, Canada), Mourad Heniche (École Polytechnique de Montréal, Canada) IC/CT2528/156

Propellants are energetic materials that play an important role in many industries such as the aeronautic (propulsion of missiles and rockets) and automobile (fast activation of air bags for car safety). In general, the production of propellant requires several unit operations. One of them, which is of interest in this study, is blending through mechanical agitation by means of so-called planetary kneaders. It is known that the investigation of mixer performance through the evaluation of

macroscopic quantities such as mixing time or power draw is a time-consuming and expensive task. 3D CFD simulation may then appear as a useful tool for the design of an efficient mixing process. However, the geometrical complexity of planetary mixers is such that standard CFD methods are just not suitable for the task. To enable simulation of fluid flow in complex geometries with internal moving parts, our research group has been developing over the past ten years finite element based fictitious domain methods that have shown both robust and accurate. The objective of this paper is to introduce our latest fictitious domain method, which is based on a fully coupled solver for the Stokes equations and which yields to a significant reduction of CPU time with respect to the previous uncoupled approach. The method is applied to the simulation of the flow of a viscous polymeric paste, typical of an industrial propellant, in a three-blade planetary mixer. The performance of the method as well as its accuracy will be discussed.

Mathematical modeling of composite patch bonding by means of induction heating. **Theodosios Papathanassiou** (National Technical University of Athens, Greece), George Tsamasphyros (National Technical University of Athens, Greece) IC/CT2413/023

Induction heating is a novel application in the field of patch bonding repair techniques. Heating with the use of induction involves placing an adhesive film, which contains a thin metal grid, between the patch and the damaged area. With the use of coils, Eddy currents are created in the metal grid, providing heat due to the Joule phenomenon. This paper focuses on heat diffusion analysis of this particular methodology. It is of major importance to have the ability of predicting the temperature distribution along composite patches during the bonding procedure. This need emanates from the fact that the structural integrity of a repair depends on several phenomena associated with temperature. Such phenomena are the curing of an epoxy matrix composite patch and the generation of thermal stresses. Simplified, Quasi 2D models of heat transfer along the patch and the plate underneath are derived from the energy conservation principle. The problem reduces to the solution of a system of ordinary differential equations. An analytical solution to the above mentioned system is derived for heating loads of polynomial distributions of random degree. This polynomial form is an adequate simulation considering the fact that any analytical function may be represented as a Taylor series expansion.

IC/CTS4650/15: General incl. microscales.

Organiser: Alexandros Sopasakis (University of North Carolina, USA)
Co-organiser: Endar Nugrahani (Bogor Agricultural University, Indonesia)

Structure and design of a vehicular-traffic model from microscopic stochastic dynamics. **Alexandros Sopasakis** (University of North Carolina, USA) IC/CT1487/015

A novel multi-lane traffic model based on stochastic noise driven dynamics is presented. The model in this work simulates vehicles under the influence of stochastic noice driven interactions. We apply an anisotropic potential and Arrhenius spin-flip and spin-exchange dynamics. This allows for highways with multiple lanes as well as entrances and exits. Vehicles advance based on the energy profile of their surrounding traffic through a novel look-ahead one-directional type interaction potential. The resulting vehicular traffic model is numerically implemented via kinetic Monte Carlo simulations and scrutinized under basic traffic flow situations.

Modeling of vehicular traffic systems. **Endar Nugrahani** (Bogor Agricultural University, Indonesia) IC/CT2995/010

The behavior of traffic systems controlled by traffic lights on a single lane is presented using the optimal velocity model. The effect of different traffic light control strategies on the traffic flow is discussed using three different strategies, i.e. the synchronized, green wave, and random offset strategies. The flow-density diagrams are analyzed using these strategies. It will be shown that the saturation of the flow occurs at the critical density, which depends on the cycle time of the traffic light and the strategy being used.

On the other hand, the behaviour of indvidual cars in a vehicular traffic system will be modelled microscopically using follow-the-leader model. The model deals with traffic flow on a unidirectional roadway in the presence of traffic lights. The responses of individual cars to red, green and yellow lights will be postulated, which gives the rules governing acceleration and deceleration of individual cars. It can be shown that only specific cars in the system are affected by the lights, while the rest behave according to simple follow-the-leader rules. In this scheme, the velocity of individual cars is determined simply by the spacing between it and the vehicle directly ahead. Finally, some simulation results on both models will be presented.

A comparison of adaptive computing and singular perturbation in the impact problem. **Lei Hou** (Shanghai University, PR China), Lin Qiu (Shanghai Jiao Tong University, PR China) IC/CT663/010

The authors applied non-linear numerical method to simulate the viscous-elastic-plastic deformation and its stress distribution . The resolution agrees with the theoretical results from the P-T/T stress PDE (Maxwell)equation. The resulting accelerations (G) have been confirmed by the celebrated European EEVC experimental solutions. Therefore the complex material stress distribution in the large deformation has been obtained. Also the posteriori-estimate solver and singular pertubation method have been used for the sensitive pre-stage deformation before the impact happening. This part of simulation is very interesting for the passive safety in automotive protection devices and airflow triggering control system. It is an important part of the mathematical modelling.

A model of drivers' lane-changing behaviour at an urban signalised intersection. **Shahrum Abdullah** (Universiti Kebangsaan Malaysia), Amiruddin Ismail (Subang Jaya, Malaysia), Ibrahim Ahmad (Univeristi Kebangsaan, Malaysia), Azami Zaharim (Univeristi Kebangsaan, Malaysia), Ibrahim bin Mohamed (University of Malaya, Malaysia) IC/CT4467/010

The aim of this research is to study and develop models for drivers' lane-changing behaviour in an urban area using the logistic regression method. A pilot study was conducted using a videotape recording technique to film an approach road leading to a signalised intersection in an urban road during the morning off-peak period. Inter-related coding methods were designed to describe and verify a driverŠs lane-changing manoeuvre. A questionnaires study to analyse the driverŠs background, experience, attitudes, lane-changing practices and their driving behaviour on the road was carried out in order to develop lane-changing behaviour models using the logistic regression method.

Calculation of effective mechanical properties of textiles by asymptotic approach. **Alexander Nam** (Fraunhofer ITWM, Kaiserslautern, Germany), Julia Orlik (Fraunhofer ITWM, Kaiserslautern, Germany) IC/CT4286/052

We consider plates with 2D periodic rod or fabric structure, used as geo-textiles or textiles. The period of structure as well as the height of the plate are much smaller compared to its depth and width. This makes a direct numerical computation of boundary value or contact elasticity problem too expensive. Two small parameters are introduced for the asymptotic analysis: the first one connected with the period of structure, the other one with the plate height.

The overcoming to the limit with respect to period of structure provides equivalent homogenized plate of the finite height. The next overcoming to the limit with respect to the height reduces the 3D problem to the membrane equations (fourth-order PDE). For the rod structures these successive formal asymptotic expansions and the algorithm for calculation of the effective elastic coefficients for the limitting homogeneous mebrane are given in[1]. In the present work, we have implemented this algorithm. We are going to justify these results by application of two-scale convergence for the first limit, and $\Gamma-$convergence for the second limit, and extend this approach and theory to textiles with sliding fibres; i.e., by adding the contact conditions in the microstructure. From the 3D homogenization (see e.g.[2]) it is known that the effective homogenized body will posess a plastic constitutive law; i.e., a nonlinear membrane equation will be obtained in the second limit.

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Transient pressure response in an anisotropic formation. **Ching-Yu Chen** (National University of Kaohsiung, Taiwan) IC/CT4504/154

The transient pressure of a single-phase is analysed here with the fluid being slightly compressible in a porous medium where a non-permeable wellbore is present. The flow is induced by a single probe on the side of an otherwise sealed wellbore which is drilled at an angle to the vertical into the anisotropic rock formation.

The formulation is derived by giving a transient correction due to the presence of the wellbore to the time dependent free space source field solution (the probe). Using the divergence theorem and the zero flux condition on the wellbore surface, a boundary element formulation is derived and solved numerically in the Laplace and Fourier transformed domain before being inverted to give the real time behaviour of the fluid pressure.

IC/CTS4655/15: Microscale, porous media.

Organiser: Oleg Iliev (Fraunhofer ITWM, Kaiserslautern, Germany)

The elasto-plastic behavior of high-performance cast alloys influenced by porosity. **Michael Ries** (TU München, Germany), Christian Krempaszky (TU München, Germany), Brigitte Hadler (TU München, Germany), Ewald Werner (TU München, Germany) IC/CT2350/154

In the design of cast high performance components, the knowledge of the effect of porosity on strength and durability is of high significance.

In this contribution, a model on the mesoscopic scale is proposed to investigate the impact of the topological aspects of the defects on the macroscopic mechanical properties of the material. In a first step only the geometrical properties of the porosity are embedded, micromechanical properties, e.g. anisotropy of the grains and influence of grain boundaries, are neglected. The constitutive behavior of the matrix is assumed to be that of the nonporous material. As a result the homogenized macroscopic behavior of the porous material is obtained. The impact of porosity is quantified by the reduction of Young's modulus, yield limit and tensile strength.

For the experimental validation of the simulations uniaxial tensile tests were conducted in a deformation dilatometer, concerning the elastic and elastoplastic properties of porous and non-porous specimens. The damage-mechanisms are investigated on broken specimens by micrographs and SEM-analysis near the fracture surface to implement them in the model in a later step. The tensile tests are conducted at room temperature and 900°C. The volume-fraction of the porosity of the specimen is obtained previously by computer tomography.

The aim is to identify adequate parameters for the description of the mechanical behavior of the porous area in a sufficient accuracy, that can be obtained by non-destructive analysis in a way as simple as possible.

A tall-block model for miscible displacement in fractured media. **Li-Ming Yeh** (National Chiao Tung University, Taiwan) IC/CT2971/154

The effects of turbulent mechanical mixing of non-stationary, incompressible, two-component, miscible displacement in a fractured medium with tall blocks is studied. In that medium, there is an interconnected system of fracture planes dividing the porous rock into a collection of tall blocks. The fracture planes form paths of high permeability. Most of the fluids reside in tall blocks, where they move very slowly. Let ϵ denote the horizontal to the vertical size ratio of the tall blocks and let permeability, gravity and width ratios of tall blocks to fracture planes be of the orders ϵ^2, ϵ^0 and ϵ^0 respectively. The equations for the two-component, miscible displacement in fractured media converge to a dual-porosity model as ϵ tends to 0. In this talk, we shall explain the dual-porosity model.

Multiscale simulation of filtration processes. **Oleg Iliev** (Fraunhofer ITWM, Kaiserslautern, Germany), Arnulf Latz (Fraunhofer ITWM, Kaiserslautern, Germany), Stefan Rief (Fraunhofer ITWM, Kaiserslautern, Germany), Andreas Wiegmann (Fraunhofer ITWM, Kaiserslautern, Germany) IC/CT4522/154

Modelling and simulation of multiple scale filtration processes is preseneted and discussed. Nano- and micron- size particles often have to be filtrated out of fluids. Filtration medium may have size of milimeters or centimeters, while a complete filter element may be of size of centimeters or meters. Proper models for each of the scales are discussed, with an emphsize on the efficient simulation approaches. The movement and the capturing of the particles is described by a stochastic ODE, while the flow of the fluid is described by Navier-Stookes, or by Navier-Stokes-Brinkman system of PDEs. Efficient solvers for complex geometries which resolve fibers of the filtration media, and for complex geometries describing a filter element, are presented and discussed.

Modelling of displacement washing of pulp fibers. **Vijay Kukreja** (SLIET, Longowal, India), Shelly Arora Shelly Arora (Punjabi University, Patiala, India), SS Dhaliwal (Punjabi University, Patiala, India) IC/CT1004/154

The flow of fluid through the packed bed of porous particles is modelled mathematically with the help of a two parameters, Peclet number and Biot number. The packed bed is divided into three parts namely, zone of flowing liquor, zone of intrapore solute present in the pores of the particles and the zone of solute adsorbed on the particle surface. Langmuir adsorption isotherm is used to describe the relationship between intrapore solute concentration and the concentration of solute adsorbed on the particle surface, whereas the bulk fluid concentration and the intrapore solute concentration are interrelated by linear adsorption isotherm. The domain across the cake thickness is divided into small sub domains called elements and with in each element the technique of orthogonal collocation is applied. The model is validated using the experimental data from a lab scale pilot plant. Indian wood pulp fibers consisting of Eucalyptus and Bamboo were used to run these experiments. The model predicted values are also compared with the experimental values.

IC/CTS4651/15: Inverse problems.

Organiser: John Stockie (Simon Fraser University, Canada)

A level-set technique for an inverse problem for Maxwell's equations in 3D. **Oliver Dorn** (Universidad Carlos III de Madrid, Spain) IC/CT2902/155

Inverse problems for Maxwell's equations in 3D play an important role in a variety of important real-world applications, for example in non-destructive testing, in mine detection, in medical imaging, in the characterization of petroleum reservoirs or in the monitoring of pollutant plumes in the Earth. The majority of inversion codes nowadays still use lower-dimensional simplifications of the full 3D system of Maxwell's equations in order to invert the data. Even though these simplified models work well in some situations of special geometry, in the general case the results they yield are not satisfactory since the problem at hand is intrinsically 3D. We will present a new technique for the identification and characterization of geophysical shapes from low-frequency electromagnetic data which uses the full system of Maxwell's equations and a 3D level set technique for solving the inverse problem. The computational cost is reduced by employing a so-called *adjoint scheme* for calculating repeated corrections for an initial guess in an iterative manner. We show that our technique is able to reconstruct and characterize hidden shapes in 3D (as for example pollutant plumes in the Earth) from relatively few noisy electromagnetic data in a stable and efficient way for realistic geophysical situations.

Level-set reconstruction from two-phase flow data incorporating statistical techniques. **Rossmary Villegas** (Universidad Carlos III de Madrid, Spain), Oliver Dorn (Universidad Carlos III de Madrid, Spain), Miguel Moscoso (Universidad Carlos III de Madrid, Spain), Manuel Kindelan (Universidad Carlos III de Madrid, Spain) IC/CT3016/155

In previous work our group has presented a novel technique for the characterization of reservoirs with more than one lithofacies which is based on a level set representation of different geological regions. In this approach the evolution of the level set function (and therefore of the geological regions) during the reconstruction is based on a gradient flow. In each step, a direct simulation and an adjoint simulation is employed in order to calculate in an efficient way descent directions of a given cost functional. If an adjoint simulator is not available, descent directions need to be calculated in a different way. In the talk we investigate and discuss alternative techniques for designing a level set evolution that does not require the use of an adjoint simulator. In particular, we will employ stochastic techniques for finding approximations or replacements of the gradient directions during the evolution of the level set function such that the final result (and therefore the final geological regions) will honor production data. We compare the performance of these adjoint-free techniques with our previous gradient based techniques. In particular, we will investigate and compare speed and accuracy of the corresponding reconstructions using realistic 2D situations with noisy production data.

An inverse Gaussian-plume approach for estimating pollutant emissions. **John Stockie** (Simon Fraser University, Canada) IC/CT1594/155

Environmental monitoring is an essential aspect of managing many large industrial operations wherein potentially harmful pollutants are potentially released into the environment. Tracking of pollutants in the atmosphere typically involves understanding a number of transport processes including turbulent and/or molecular diffusion, advective transport by the wind, and deposition on the earth's surface. The Gaussian plume model is a steady state model which yields a simple analytical solution to the atmospheric transport equations that depends linearly on the emission rate, Q. The Gaussian plume solution has been used to great advantage in developing industry-standard software packages that track pollutant emissions for known Q; however, relatively little work has been done on the inverse problem, namely estimating Q given measurements of particles deposited on the ground surface.

I will present a study of a large mining operation which involved estimating pollutant emission rates for several sources distributed spatially over an actual industrial site. A linear least squares optimization approach is employed to estimate the sources, and the ill-conditioning of the inverse approach is discussed. A forward solver for integrating the unsteady atmospheric transport equations – based on the high resolution algorithms implemented in CLAWPACK – is also proposed to validate the results.

This project is joint work with Ed Kniel (Teck Cominco Ltd.), Enkeleida Lushi (NYU), and Evgeniy Lebed (UBC).

Variational approach to the inverse identification of cracks from boundary measurements. **Rumena Tsotsova** (Universität Karlsruhe, Germany) IC/CT2638/155

This study presents a variational method for identification of internal cracks in isotropic homogeneous body. The method is based on measurement data collected on the boundary of the solid (displacement and traction fields). The determination of the crack position, topology and shape can be considered as a free-discontinuity problem with the unknown pair $(\mathbf{u}, K)$, where $\mathbf{u}$ represents the displacement vector in the unfractured part of the body and K the crack surface.

To obtain the solution pair $(\mathbf{u}, K)$ a functional, based on the variational formulation provided by Mumford and Shah [1] can be utilized. The variational relaxation with elliptic lower semicontinuous functional of the primal variational formulation proposed by Ambrosio and Tortorelli [2] Γ-converges to the strong discontinuity problem of static fracture mechanics (non-propagating crack) and by finite element method, it can be numerically minimized with respect to $\mathbf{u}$ and the defect parameter ϕ. The defect parameter is a $\mathbb{H}^1$-function on the reference placement of the solid body with values in the interval $[0, 1]$ and can be interpreted as a smooth indicator for the states between: *crack* ($\phi = 0$), and *solid* ($\phi = 1$).

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A Mathematical model for a nonlinear soil-column experiment. **Gongsheng Li** (Shandong University of Technology, PR China), De Yao (Shandong University of Technology, PR China), Yongji Tan (Fudan University, PR China), Hongliang Liu (Shadong University of Technology, PR China) IC/CT2815/155

This paper deals with a one-dimensional soil-column experiment and its mathematical models. Due to the nonlinear behaviors of solute transportation in soils and groundwater, the ordinary retardation factor could be a nonlinear function of solute concentration, and the zero production term could be modified to a nonlinear term related with the time and solute concentration, and then a new mathematical model is put forward for nonlinear soil-column experiments. Furthermore, a real soil-column experiment in Zibo, Shandong Province is investigated, and an inverse problem of determining the source coefficients of the model is set forth according to the additional data of breakthrough curves (BTCs). By applying an optimal perturbation algorithm instead of regularization strategies, the source coefficient is determined both in the cases of accurate data and noisy data. The computational results show that the optimal perturbation algorithm is efficient at least in the problem of this paper, and the mathematical model here could be applied to explore some soil-column experiments with nonlinear transport behaviors.

3D complex structures imaging based on acoustic wave equation. **Wensheng Zhang** (Chinese Academy of Sciences) IC/CT801/155

Structures imaging is an important data processing step to detect oil reservoir in oil geophysical exploration. In the point of mathematical view, it solves an initial value problem of acoustic wave equation. In this paper, the hybrid imaging method based on 3D acoustic wave equation is investigated, and some new corresponding computational schemes are proposed. Firstly, the 3D full-way acoustic wave equation is decomposed into a coupled system of one-way wave equations, which describes the propagation of downgoing wave and upcoming wave. In order to obtain images of structures, the known-data which recorded on the surface (initial data) are required to extrapolate along depth or travel-time direction. The extrapolating equations for the downgoing wave and upcoming wave are the uncoupled one-way equations, which is an approximation of the coupled system under the assumption of neglecting multiple reflections. Secondly, the hybrid method and its computational schemes for solving the one-way equations are derived. The hybrid method extrapolates wavefield in the frequency-space domain with the finite-different method and in the frequency-wavenumber domain with the fast Fourier transform (FFT) alternatively, and it possesses the advantages of high imaging accuracy. Two kinds of extrapolating algorithm are considered. One is the two-way splitting scheme, which extrapolates wavefield along two perpendicular directions alternatively. The two-way splitting scheme contributes to solving two tri-diagonal equations successively and has the virtue of high computational efficiency. However, it may cause azimuth numerical errors. The other is the four-way splitting scheme, which extrapolates wavefield along four different directions alternatively. The four-way splitting scheme may reduce the numerical anisotropic errors caused by the two-way splitting scheme. All schemes and the relevant error analysis are given. Thirdly, the numerical calculations both for a pulse response and a complicated benchmark model are completed. Since the 3D wavefield extrapolation is a large scale computational problem, parallel programming based on the Message Passing Interface (MPI) is used to improve computational efficiency. The computational codes are performed on PC cluster and high parallel efficiency is obtained. It is noted that the proposed algorithm can yield accurate images for 3D complex structures.

Key words: 3D, acoustic wave equation, finite-difference method, FFT, imgaing/inversion, parallel computation

IC/CTS4654/15: Fluids.

Compositional space parameterization for multi-component multiphase flow in reservoirs. **Denis Voskov** (Stanford University, USA), Hamdi Tchelepi (Stanford University, USA) IC/CT3049/156

We describe a robust and computationally efficient method for large-scale compositional reservoir simulation involving large numbers of components (e.g. gas injection processes). In the standard compositional simulation approach, an Equation Of State (EOS) is used to describe the phase equilibrium. For each gridblock, given the temperature, pressure and overall compositions, the EOS is used to detect the phase state (e.g., one, two, or three phases), and if multiple phases are present, calculate the phase compositions. These EOS computations can dominate the overall simulation cost. This is especially the case for simulations of gas injection processes involving large numbers of components (five or more) in highly detailed reservoir models.

We propose a different approach based on compositional space parameterization (CSP) in terms of the tie-lines. This approach makes full use of the improved theoretical understanding of compositional gas-injection processes developed by Orr and co-workers over the last two decades. In the CSP simulation method, the basic idea is to represent any composition in the tie-line space using (1) a set of parameters, which determine uniquely the tie-line that intersects this composition, and (2) the overall concentration of one component, which locates the specific location of the mixture composition on the tie-line. The CSP based algorithm has been implemented in a general-purpose research simulator. Using several challenging compositional simulation problems of practical interest, we demonstrate the robustness and superior computational efficiency of the CSP method. Our computational experience indicates that the CSP approach is (at least) an order of magnitude more efficient than standard EOS-based simulations.

Parameterization for mesoscale ocean transport through random-flow models. **Banu Baydil** (Rensselaer Polytechnic Institute, USA), Peter Kramer (Rensselaer Polytechnic Institute, USA), Shafer Smith (New York University, USA) IC/CT4123/156

We describe a mathematical approach based on homogenization theory toward representing the effects of mesoscale coherent structures, waves, and turbulence on large-scale transport in the ocean. We are developing a systematic parameterization strategy by building up deterministic and random subgrid-scale flow models in an increasing hierarchy of complexity, coupling the results from numerical simulations of cell problems with asymptotic analysis with respect to key nondimensional physical parameters such as Peclét and Strouhal numbers.

A two immiscible liquids penetration model for surface-driven capillary flows. **Riccardo Fazio** (Università degli Studi di Messina, Italy), Giovanni Cavaccini (Alenia Aronautica, Italy), Vincenza Pianese (Alenia Aronautica, Italy), Salvatore Iacono (Università degli Studi di Messina, Italy), Alessandra Jannelli (Università degli Studi di Messina, Italy) IC/CT865/156

At the beginning of the nineteen century Young and Laplace, working independently, were the first to report on theoretical studies concerning surface tension and capillarity. Their work, made approximatively at the same time, reported that the static pressure on the liquid side of the liquid-air interface is reduced by the effect of the surface tension. Later, Hagen and Poiseuille, studied the flow of viscous liquids in circular pipes (and capillary tubes in particular), derived the well-known Poiseuille flow profile for a laminar, fully developed, Newtonian fluid. Reynolds tested experimentally the stability of the Poiseuille profile, finding that it held in the case of laminar flow. The dynamics of liquid flow into a capillary, has been modelled by the classical Washburn equation, the Bosanquet model, and, more recently, the SNC model (by Szekely et al.). Applications of surface tension driven capillary flows range from liquid penetration in non-destructive tests to porous membrane and substrates absorption in medicine and personal care. Our main concern is to define a two immiscible liquids penetration model. Moreover, we would be interested to study horizontal closed-end capillaries. In this context, the effect of the entrapped gas on the liquid dynamics was investigated, first, by Deutsch from a theoretical viewpoint, and, more recently, by Pesse et al. from an experimental one. At the end of the presentation several numerical simulations will be reported.

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Multigrid fictitious-boundary and grid-deformation methods for flow-induced rotation of wing. **Decheng Wan** (Shanghai Jiao Tong University, PR China) IC/CT2310/156

Flow-induced rotation of wing in incompressible viscous flows are often met in aero- and hydro- dynamics. For example, an airfoil that has a fixed center of mass can be induced to rotate freely around its center of mass due to hydrodynamic forces under the action of an incoming incompressible viscous flow in a channel. It is quite hard to simulate the flow induced rotation of wing in incompressible viscous flows, since different differential equations must be satisfied on each side of the interface between fluid and wing and the solutions are coupled through relationships or jump conditions that must hold at the interface. The movement of both the interface and the wing is unknown in advance and must be determined as part of the solution, it can require a huge amount of time for the generation of a boundary-fitted mesh for each different position of the moving wing. In this paper, numerical simulations of flow-induced rotation of wing by multigrid fictitious boundary and grid deformation methods are presented. The flow is computed by a special ALE formulation with a multigrid finite element solver. The solid wing is allowed to move freely through the computational mesh which is adaptively aligned by a special mesh deformation method such that the accuracy for dealing with the interaction between the fluid and the solid wing is highly improved. The advantage of this approach is that no expensive remeshing has to be performed, and the accuracy for capturing the surfaces of solid wing is highly preserved since the grid points are concentrated near the surfaces of the wing. Here, only the solution of additional linear Poisson problems in every time step is required for generating the deformation grid, which means that the additional work is significantly less than the main fluid-solid part. Several numerical examples of 2D flow around free rotation wing in a channel are provided to show the efficiency of the presented method.

Microcomputer-based simulation of heat conduction between solid of tapered shape and the fluid. **Purnima Shrivastava** (Patna University, India) IC/CT3984/156

Simulating the heat conduction in between a solid conducting body immersed in fluid at a given temperature is a difficult task, particularly when the body is tapered in shape and the simulation is to be carried out on microcomputer. The writer has worked in the past on particular solutions through analytical methods and has encountered the practical difficulties arising out of numerical modelling.

The body in question is cylindrical, symmetrical about z-axis, of length l, tapered in shape and has been heated to a high temperature before being immersed into fluid (water at 50deg. c).The heat conduction equation in polar coordinates is attempted to be solved in two ways- first analytically making use of Bessel's function. A specific solution has been obtained as the boundary conditions are all derivatives of temperature w.r.t. either radius or height.

Secondly, the numerical modelling has been attempted with the help of Finite Difference method. Attempt has been made to solve the equations thus formed through ADI implicite scheme on microcomputer, which seems difficult due to large memory requirements. A change in algorithm is required.

The talk seeks to give an account of work already done on this and would include further possibilities for general solution under the all derivative boundary conditions with analytical methods and for a suitable numerical solution on microcomputer (for a low- cost solution). Also, any possible analogy with flow of fluids shall be discussed.

Positive 2D hybrid linear systems. **Tadeusz Kaczorek** (Politechnika Warszawska, Poland) IC/CT3312/015

Abstract: A new class of positive hybrid linear systems is introduced. The solution of the hybrid system is derived and necessary and sufficient condition for the positvity of the class of hybrid systems are established. The classical Cayley-Hamilton theorem is extended for the hybrid systems. The reachability of the hybrid system is considered and sufficient conditions for the reachability are established. The considerations are illustrated by a numerical example.

15: Modelling and Simulation, Posters

IC/PP4288/096: **Modeling and simulation of suction caisson: a study of plastic analysis theory.**

Presenter: Hooman Monajemi (University of Malaya, Malaysia)
Co-author: Hashim Abdul Razak (University of Malaya, Malaysia)

Suction caisson foundation are subjected to different combination of horizontal, vertical and moment loadings depending on the type of structure which they are used for. In addition the optimum ultimate capacity of the suction caisson subjected to the combined loading depends on a variety of parameters such as caissons aspect ratio, soil property and etc. The skirt length to the diameter ratio (L/D) is generally less than 1 for fixed structures like jacket platforms or wind turbines and more than 1 for the suction caissons used as anchors in tension leg platforms (TLP) or floating structures. For large values of L/D they

are sometimes referred to as suction piles. The behavior of the suction caisson subjected to lateral loading is presented in this paper using plastic limit analyses (PLA) method and finite element simulation. This is to observe the effects of aspect ratio (L/D) and soil properties to the failure mechanism and lateral ultimate capacity of the foundation. A combination of horizontal and rotational reaction due to the lateral loading is considered and the ultimate capacity of the foundation for the combined horizontal moment loading is elaborated. This can be done by applying combination of horizontal displacement and rotation to the suction caisson. The general purpose finite element program DIANA is being used for this study. A non-linear analysis was performed on a three dimensional model formed using eight- node isoparametric solid brick elements. The soil was modeled as an elastic perfectly plastic material with Von Mises yield criterion for saturated clay. The plastic limit analyses (PLA) is an upper bound plasticity formulation which is base on calculation of the rate of internal energy dissipation equate to the rate of work due to the external loads. The ultimate load capacity calculated from PLA methods can be use as a benchmark to evaluate the accuracy of FEM solutions.

IC/PP4379/015: Continuous solutions in boundary-layer problem.

Presenter: Aliona Dreglea (Dublin Institute of Technology, Ireland)

Let us consider the following BVP:

$$\begin{cases} x'''(t) + M(x(t),t)x''(t) = 0\,,\ \alpha < t < \beta\,, \\ x(\alpha) = a\,, \quad x'(\alpha) = b\,, \quad x(\beta) = c\,. \end{cases}$$

Some problems from the theory of boundary layer in fluid dynamics [1–2], can be reduced to mentioned problem. Let a function $M(x,t)$ be defined and continuous in the area

$$D = \{x,t|\ |x| \le |a| + |b|\,|\beta| + |c - a - b\beta|\,,\ \alpha \le t \le \beta\}\,,$$

$$m = \min_{x,t\in D} M(x,t)\ \ M = \max\left\{\max_{x,t\in D} M(x,t), 0\right\}$$

In special case $\max M(x,t) = x$, $\alpha = 0$, $\beta = 1$ in the monograph [3, pp.412–413)] existence of a solution has been proven. In this talk we proof the solution existence for this BVP on a finite interval $[\alpha,\beta]$. The function $M(x,t)$ can be any continous function satisfying the condition A.

THEOREM. Let condition A be satisfied. Then the BVP on the $[\alpha,\beta]$ has solution the class $C^{(3)}_{[\alpha,\beta]}$.

[1] Schlichting H.; Boundary Layer Theory, 7th edition, McGraw Hill, (1951).

[2] Landau L.D. and Liftshitz E.M.; Fluid Dynamics, Moscow. Nuaka, (1988).

[3] Trenogin V. A.; Functional Analysis, Moscow, Nauka, 1980.

IC/PP4517/015: Mathematical and computational modelling for biosensor: a modular approach.

Presenter: Yupeng Liu (Dublin, Ireland)
Co-author: Qi Wang (Dublin, Ireland)

Biosensor are analytic devices which detect biochemical and physiological changes and represent an emerging technology for low-cost , rapid and simple to operate biomedical diagnostic tools.Biosensor has become very significant to our daily life in many areas, home-testing devices for many diseases and disorders, measuring water quality, presenting the harmful microorganisms in food etcs.Biosensor design underpins the development of a range of next generation biomedical diagnostic tools which will directly affect the quality of life worldwide over the next few decades.Using mathematical and computational modeling techniques to characterize the biosensor response as a function of its input parameter in wide range of physical contexts, it can guide experiments, therefore reducing development times and costs.Modular approach of modeling aims to investigate the problem of optimizing biosensor design using an interdisciplinary approach which combines mathematical and computational modeling eighth electrochemistry and biochemistry techniques.Specifically , a collection of simple models will be developed and the used as building blocks towards descrying more complex electrochemical immunoassay systems.The ultimate goal envisaged is the develop a flexible, modular mathematical model, implement in C programming language, which can be used towards a software platform capable of predicting the behavior of a wide range of electrochemical and optical biosensor.

IC/PP476/010: Temperature field of solid body, incorporating cylindrical channel with thermally-thin layer under pulse modes of heat exchange with environment.

Presenter: Nikolay Belyakov (BMSTU, Moscow, Russian Federation)

Using the method of generalized integral transformation and the idea of kernel splitting, an approximate analytical method to solve the appropriate boundary problem for the unlimited solid isotropic body, incorporating a cylindrical channel with thermally-thin surfacing is developed. Special attention is given to the problem of pulse modes of heat exchange. The influence of the thermally-thin layer on temperature field is studied.

IC/PP4695/151: Electromagnetic models of magnetic-flux leakage inspection of steel products.

Presenter: Javier Etcheverry (Tenaris, Argentina)

Magnetic flux leakage (MFL) is one of the most widely used techniques for non-destructive inspection of steel pipes. There are several different equipment designs that specialize to the detection of longitudinal, or transversal, or surface defects. It is also possible, sometimes, to infer the location of the defect from the form of the MFL signal. In order to achieve a better defect detection and improve the classification, it is important to investigate how the detected signal depends on the relevant parameters (location and shape of the defect, excitation field intensity, magnetic properties of the inspected material, etc.).
We will report results for the non-destructive inspection of steel pipes obtained from 2D nonlinear magnetic simulations (using finite element techniques), and present 3-D computations using a coupling between boundary elements (to approximate the problem in the air and non-ferromagnetic materials) and finite elements for the steel. This later approach provides a formulation where only ferromagnetic parts need to be meshed, thus simplifying the set-up of the complex geometries involved. The presented model considers the possibility of including complex nonlinear or hysteretic behavior of the material, thus allowing to evaluate final magnetization states, demagnetization strategies, etc.
This work was done in collaboration with Gustavo Sánchez and Tomás Guozden.

IC/PP2631/156: Assesment of several depth averaged turbulence models for computing turbulent free surface flow in hydraulic structures.

Presenter: Luis Cea (Universidade da Coruña, Spain)
Co-author: M. Elena Vazquez-Cendon (Universidade de Santiago de Compostela, Spain)
Co-author: Luis Pena (Universidade da Coruña, Spain)
Co-author: Jeronimo Puertas (Universidade da Coruña, Spain)

The depth-averaged shallow-water equations have been extensively used in order to model the flow in rivers and coastal regions, flooding and drying problems, and shallow free surface flows in hydraulic structures. The equations assume a vertical length scale much smaller than the horizontal one, which reduces the vertical momentum equation to the hydrostatic pressure distribution. At the same time the velocity field is assumed to be uniform along the vertical direction. Both assumptions are reasonably fulfilled in rivers and coastal regions. However, quite often in hydraulic structures the separation of scales assumption is not fulfilled, at least in some regions of the flow, due to 3D local flow patterns and high turbulence levels. Therefore, it is of most importance to verify with experimental data the quality of the numerical results in different types of hydraulic structures.

In this paper the free surface flow in several hydraulic structures is computed with a depth averaged shallow water model coupled with several turbulence models, which include a mixing length model, a $k-\varepsilon$ model, and an algebraic stress model. In order to take the equations to their limits of application, we have studied flows with a high turbulence intensity, in which the implicit assumptions of the 2D-SWE are partially broken in some regions of the flow. This is specially interesting in order to verify the quality of the numerical results under such *extreme* flow conditions. The flows studied include several designs of small hydros, two designs of vertical slot fishways, and an open channel with a 90^o bend.

In all cases, the numerical velocity and turbulent fields are compared with comprehensive experimental results.

IC/PP41/015: Modeling risk in arbitrage strategies using finite mixtures.

Presenter: Adam Tashman (Stony Brook University, USA)

Arbitrage strategies produce stable, modest returns punctuated by intervals of dramatically poor performance. The weakness stems from an oversight in modeling: seemingly independent bets infrequently become highly correlated to market variables. Thus, the risk in arbitrage strategies is systematically underestimated, and hedging is not properly implemented. A set of arbitrage strategies are examined for evidence of a mixture of distributions. When such structure exists, a finite mixture model is fit to explain the states of high and low correlation. The model uses a logistic regression function for the mixture probability and linear regression functions for the component densities. The covariates considered are stock market return (SP500), volatility (CBOE VIX), swap spread, and credit spread. The dependent variables are index returns for event arbitrage, statistical arbitrage, and convertible arbitrage. The model is applied in a novel hedging strategy, termed mixture hedging. The strategy is back tested over the period 1990-2005, whereby rolling 12-month returns are computed. Event- and convertible arbitrage exhibited evidence of a mixture, while statistical arbitrage did not. The mixture model better explained periods of negative performance than regression analysis. Mixture hedging applied to event arbitrage admitted a maximum drawdown of -0.78 percent, compared to -1.10 percent for the unhedged portfolio. The results indicate that mixture models better capture the regime-switching nature of arbitrage returns, and offer an improved method for hedging risk.

16: Pure Mathematics, Minisymposia

IC/MP521/162: **Topological robotics.**

Organiser: Michael Farber (University of Durham, UK)
Co-organiser: Robert Ghrist (Univ. of Illinois at Urbana-Champaign, USA)
Co-organiser: Daniel Koditschek (University of Pennsylvania, USA)

Topological robotics is a new and rapidly growing area of applied mathematics which uses techniques and perspectives from modern topology in the service of robotics problems.

Topological robotics studies topology of configuration spaces of various mechanisms (e.g. linkages) and applications to control theory which use topology of underlying configuration spaces. The scope of directions of topological robotics includes the theory of robot motion planning algorithms and their applications to collision free control of multiple moving objects. Some important aspects of topological robotics deal with problems of design of specific dynamical systems exhibiting prescribed behavior (modelling autonomous robots moving in various environments). Topological robotics uses methods of modern algebraic topology, Morse theory and the theory of dynamical systems. Combinatorics and the theory of subspace arrangements also play an important role. Recently, methods of geometry on spaces of nonpositive curvature were successfully employed. The talks of the mini-symposium represent several central directions of topological robotics.

Algebraic topology for networks. **Robert Ghrist** (Univ. of Illinois at Urbana-Champaign, USA) IC/MT3528/0

This talk will explain new applications of algebraic topology to problems in networked systems. A typical network of sensors or robots has the goal of monitoring a given environment. With the use of numerous cheap 'local' devices comes the problem of integrating local environmental data into a global picture via (typically wireless) communication links. This integration problem is remarkably amenable to the tools of algebraic topology, especially homology theory and Euler characteristic. The talk will give all the requisite background and provide concrete applications of computational topology to problems involving coverage, hole detection and repair, pursuit and evasion, and target enumeration.

The cohomology ring of chain and polygon spaces. **Jean-Claude Hausmann** (Université de Genève, Switzerland), Michael Farber (University of Durham, UK), Dirk Schütz (University of Durham, UK) IC/MT2463/0

We prove that chain-spaces in R^d (and polygon spaces for $d = 2, 3$) are determined by their cohomology rings.

Betti numbers of random manifolds. **Michael Farber** (University of Durham, UK), Thomas Kappeler (Universität Zürich, Switzerland) IC/MT2117/0

In various fields of applications, such as topological robotics, configuration spaces of mechanical systems depend on a large number of parameters, which typically are only partially known and often can be considered as random variables. Since these parameters determine the topology of the configuration space, the latter can be viewed in such a case as a random manifold. We study mathematical expectations of Betti numbers of random manifolds in the special case of planar linkages, viewing the lengths of the bars of the linkage as random variables. Our main result gives an explicit asymptotic formulae for the mathematical expectations of the Betti numbers for two distinct probability measures describing the statistics of the length vectors when the number of links tends to infinity.

The construction of vector fields for programming work. **Daniel Koditschek** (University of Pennsylvania, USA) IC/MT3712/0

The problem of robot motion planning has stimulated a three decade old literature addressing the construction of paths joining pairs of points in a robotic Şfreespaceť (the topological space arising from the safe placements of a robot in its intended physical environment). The problem has been shown to be hard from a number of different viewpoints. Most recently, Farber and colleagues have used classical techniques of topology to show that continuous motion planners cannot exist over most freespaces of practical interest, and have developed estimates for the minimal number of components into which such planners must be decomposed in a growing number of relevant cases.
When a robot is required to perform some work within its environment then it is most natural to seek a planner taking the form of a vector field (or, more generally, a family of hybrid dynamical systems) whose attractors satisfy the predicates characterizing desired goal conditions and whose repellors include any states with unsafe or otherwise forbidden properties. This problem has received far less attention in the literature. There are relatively few constructive methods available and the fundamental limitations are not yet well characterized.
This talk will review the general problem of programming work, provide some practical examples of successful constructions, and speculate on the nature of the fundamental limitations.

16: Pure Mathematics, Contributed Talks

IC/CTS4899/16: **Pure mathematics.**

Singular initial-value problems for functional-differential equations: solvability, number of solutions, asymptotics. **Oleksandr Zernov** (South Ukrainian State Pedagogical University) IC/CT792/163

We will speak about linear, perturbed linear and nonlinear equations. Also we will speak about hybrid systems which contain both regular and singular systems, or which contain subsystems with distinct types of singularity. We find solutions with required asymptotic properties by means of quilitative methods. Most of the results are new and have not been published before.

On conformal mappings of spherical domains with given scale functions. **Ludmila Bourchtein** (Universidade Federal de Pelotas, Brazil), Andrei Bourchtein (Universidade Federal de Pelotas, Brazil) IC/CT1366/163

One of the most widespread approaches to planar representation of the Earth surface, required in different problems of geophysics, geodesy and cartography, is conformal mapping. To measure the degree of distortion caused by a projection of the spherical domain Ω onto a plane, the distortion coefficient $\delta(\Omega) = \sup_\Omega m / \inf_\Omega m$ can be used, where m is the scale function defined as the ratio between the elementary arc lengths along a planar curve and respective spherical curve. The distortion coefficient represents the quantitative evaluation for both cartography distortion and computational grid efficiency because the number of time steps of an explicit or semi-implicit scheme implemented on a δ-distortion grid increases δ times as compared with implementation on "ideal" physically uniform grid with $\delta = 1$.

One of the open problems in flattening the sphere surface is the construction of the conformal mappings with prescribed properties of scaling, in particular, the problem of finding the projections with the minimum possible distortion. In this study, the problem of finding the conformal mapping from a sphere onto a plane with a given scale function independent of longitude is solved for an arbitrary spherical domain. The obtained results are compared with the well-known projections used in cartography and geophysical fluid dynamics. The problem of minimization of the distortion under conformal mappings is solved for domains in the form of the spherical disk. The efficiency of the computational grids based on the minimum distortion projections is evaluated in comparison with conventional grids.

On some generalizations of the classical Riemann problem and its corollaries. **Irina Dmitrieva** (South Ukrainian State Pedagogical University) IC/CT525/163

We are looking for a function $F(z)$ that is analytic everywhere on complex plane or on any other algebraic surface of nonzero genus excepting not the obligatory finite set of the ramification points. The function's values undergo the corresponding permutations when passing round these points, and $F(z)$ is assumed to have a finite order at infinity.

Here the following moments have to be underlined: in the classical statement of Riemann problem the set of ramification points was the finite one, all the appropriate permutations were of one and the same dimensions and the unknown function was sought on complex plane [Riemann, B., Gessamelte Mathematische Werke, 2. Aufl., Teubner, Leipzig, 1892]. In our case the proposed problem is investigated not only on complex plane, but on any algebraic surface of finite genus, though this fact is not a principal one here, because some results in this direction were obtained earlier [Dmitrieva, I. Yu., Factorization of Noncom. Permut. Matrices on an Algebr. Surf. of Nonzero Genus, St. Petersburg Math. J. 4(1993), No. 2, 309 - 318].

The most important facts, that considerably differ from the classical statement, in our case consist of : 1) the set of ramification points is not obligatory a finite one:; 2) to every ramification point corresponds the permutation of its own dimension, i.e. the permutations' orders are not equal to each other. Therefore, we obtain here the generalization of the notion of Riemann surface not only in the classical sense, but also as a new aspect for the algebraic surface covering.

At the same time we have come to the homogeneous vector boundary Riemann - Hilbert problem in the new terms and with the special construction of the permutative matrix coefficient.

Relevant applications concern mostly the field theory.

Non-local Dirichlet forms generated by pseudo-differential operators on compact Abelian groups. **Emil Popescu** (Technical University of Civil Engineering, Romania) IC/CT2977/163

Let G_i, $1 \leq i \leq n$, be compact abelian groups and let Γ_i, $1 \leq i \leq n$, be countable dual groups. We consider $G = G_1 \oplus G_2 \oplus ... \oplus G_n$ and $\Gamma = \Gamma_1 \oplus \Gamma_2 \oplus ... \oplus \Gamma_n$. For $1 \leq j \leq n$, let a_j be a negative definite function on Γ_j and $a(\gamma) = \sum_{j=1}^n a_j\left(\gamma_j\right)$. For $\varphi \in S(G)$, the set of all generalized trigonometrical polynomials on G, we define $L\varphi(x) = \sum_{j=1}^n b_j\left(x_j'\right) A_j \varphi(x)$, where $\widehat{A_j\varphi}(\gamma) = a_j\left(\gamma_j\right)\hat{\varphi}(\gamma)$, $1 \leq j \leq n$. Then $B(\varphi,\psi) = \sum_{j=1}^n \int_G b_j\left(x_j'\right) A_j^{1/2}\varphi(x)\overline{A_j^{1/2}\psi(x)}\mathrm{d}x$ is a Dirichlet form with the domain $H_a^{1/2}(G) = \left\{u \in L^2(G) \mid \sum_{\gamma\in\Gamma}(1+a(\gamma)) \mid \hat{u}(\gamma)\mid^2 < \infty\right\}$ on $L^2(G)$. The properties of fractional powers of continuous negative definite functions and their corresponding Dirichlet forms are also investigated.

Induced topology on fuzzy singletons. **Velu Lakshmana Gomathi Nayagam** (NIT Tiruchirappalli, India), Geetha Sivaraman (Thiagarajar College, Trichy, India) IC/CT4532/162

The notion of fuzzy sets was introduced by L.A. Zadeh (1965). The notion of fuzzy topological spaces was introduced and studied by C.L.Chang (1968). The notion of fuzzy singletons is introduced by Pao and Liu (1980). In this paper the notion of induced topology on the collection of fuzzy singletons with respect to a fuzzy topological space is introduced and studied. The relation of the existing notions of Fuzzy separation axioms, Fuzzy compactness and Fuzzy connectedness with the notions of Separation axioms, Compactness and Connectedness in this topology have been studied.

What is really the differential? the fundamental concept of calculus. **José Manuel Olivencia Quiñones** (Universidad Nacional de Trujillo, Peru), Orlando Martín Hernández Bracamonte (Universidad Nacional de Trujillo, Peru) IC/CT874/017

The use of the differential concept is necessary, frequent but poorly understood. Our preoccupation is not centered in the purely mathematical sense, but also in its applications. The differential concept is usually relegated in the teaching of the mathematics, by the contrary, is very useful in the reasoning and mathematical formalization of applied situations. Since the birth of the differential calculus to current time, the differential concept was debated between its identification with the infinitely small amounts and their reduction to a subordinated expression without own meaning (the differential of Newton and Leibniz and later the differential of Cauchy).

In this work, a clarification is carried out, that is able to reconcile, on the one hand, the close relation with the applied situations of the differential expressions of Newton, Leibniz and Cauchy, and, on the other hand, the rigour and the precision of its meaning, achieving a suitable and useful understanding of the differential concept. For it, we simply use the differential definition like a linear transformation and conceiving it like so, working in the space of the linear transformations, it is perceived with great clarity that the differential, instead of being an infinitesimal increase, it is the best linear approximation of the variation of a function at a point, furthermore, it is the unique linear estimation that, via integration, produces the exact relation between the variation of the independent variable and the variation of the dependent variable. In our experience, this conception is producing encouraging results. It is even established, of a very natural way, a differential algebra, that allows performing operations with the differentials, with great facility, maintaining the intuitive sense and without losing the obtained clarification.

16: Pure Mathematics, Posters

IC/PP1253/010: On applications of q-fractional calculus.

Presenter: Sunil Purohit (Udaipur, India)
Co-author: Rajendra Yadav (DEPARTMENT OF MATHEMATICS & STATISTICS, J. N. VYAS, India)

The object of this paper is to illustrate how the q-fractional calculus approach can be employed to derive a transformation expressing a generalized basic hypergeometric function in terms of a finite sum of lower order functions. A further generalization of the main result is also deduced. Known results due to Karlsson, P.W. [J. Math. Phys., 12 (1971), 270-271] and Raina, R.K. [Rend. Sem. Mat. Univ. Padova, 83 (1990), 7-12] follows as the limiting cases of the main results.

IC/PP3066/163: Quasi-conformal extension of biholomorphic mappings in several complex variables.

Presenter: Paula Curt (Universitatea Babeş-Bolyai, Romania)
Co-author: Gabriela Kohr (Universitatea Babeş-Bolyai, Romania)

In this work we present sufficient conditions for the first element of a Loewner chain to be extended to a quasiconformal homeomorphism of $\overline{\mathbb{R}}^{2n}$ onto itself. Interesting applications will be also considered.

IC/PP2932/163: Modern and recent contributions in the theory of Loewner chains of several complex variables.

Presenter: Gabriela Kohr (Universitatea Babeş-Bolyai, Romania)

In this work we present modern contributions in the theory of Loewner chains and the Loewner differential equation in several complex variables. Interesting applications will be presented.

IC/PP4162/163: A study of unified finite integrals and expansion formulae for the $\bar{H}$ function, with application.

Presenter: Anil Ramawat (JODHPUR, India)

In this paper we establish one single integral and two multiple integrals involving product of extended Jacobi polynomials, general class of polynomials and the $\bar{H}$ function. These integrals are unified in nature and act as a key formulae from which we can derive as its particular cases, integrals involving a large number of simpler special functions and polynomials. For the sake of illustration, we gave here only one particular case of our first integral which is also new and of interest by itself. An expression formula for the $\bar{H}$ function, in a series involving products of the $\bar{H}$ function and generalized LegendreŠs associated functions is also established. The generalized LegendreŠs associated functions reduce to associated Legendre function on setting $m = n$. Also, on specializing the parameter of the $\bar{H}$ function in the expansions, we may get many interesting expansions. At the end, we give an application of our first integral by inter-connecting them with the Riemann–Liouville type of fractional integral operator.

17: Education Culture and History, Minisymposia

IC/MP179/171: E-learning and remote access tools in applied mathematics.

Organiser: Matti Heilio (Lappeenrannan Teknillinen Yliopisto, Finland)

The cutting edge knowledge in mathematical technology in Europe is found dispersed at small nodes. Virtual environments can be used to bring solutions to training, education and research, to facilitate distributed work processes, provide remote access to knowledge repositories etc. We are focusing on the challenge of using web-based solutions in education of modelling and applied mathematics. We envisage a possibility of a European digital environment, a menu of courses and remote access software tools, built on the concepts of current e-learning technologies.

Topics on the talks include Distant learning in mathematical modelling, Web-tool on differential equations, Remote courses for applied mathematics in the Third World universities, Learning objects and blended learning in web-supported education.

Distant learning in mathematical modelling in Finland. **Seppo Pohjolainen** (Tampereen Teknillinen Yliopisto, Finland) IC/MT3743/171

Department of Mathematics at Tampere University of Technology is coordinating a national network project on mathematical modelling. Ten universities and research institutes are participating in the network project and the teachers of these universities are responsible for certain parts of the courses produced. Students from different universities can study mathematical modelling both individually and collaboratively.

In the project Web-based learning and teaching methods have been developed, content production in mathematical modelling has been supported and administrative measures needed to support web-based learning and teaching have been put into practice.

In the presentation experiences obtained from course planning, courseware production, pedagogy, didactics, technology and student feedback will be presented and analysed in detail.

Learning objects and blended learning in web-supported education. **Helle Rootzen** (Danmarks Tekniske Universitet, Denmark) IC/MT3850/171

Students nowadays differ much more than before; some are very good and some have substantial difficulties even with very basic concepts. *Learning Objects* may be used to ensure that each student gets course material which is at the right level. Further, students have very different learning styles; some learn best by first getting exposed to theory and afterwards seeing examples, while others prefer the opposite order of presentation. Similarly some prefer visual and graphical teaching, some like to see theory written down in formulas, while others get the most out of listening to oral presentations. Learning Objects make it possible for each student to use what suits her best.

Faced with a new generation of students who are used to exploiting the possibilities of the computer, we need a new type of education that will reflect a rethinking of content, form and duration. In the future, education will be in the form of *voucher systems*. You get a set of vouchers and use them to attend the specific chunk of a study programme you need whenever and wherever it suits you. If the providers are to meet these requirements, the task of developing new courses and tailoring these to new students must be manageable. We therefore propose a new type of courses. These are structured around Learning Objects, short complete education sessions, which may be combined in various ways according to the student's interests and levels. We use blended learning where we combine Learning Objects with face-to-face sessions. The ideas are tried out in research-based continuing education in applied statistics.

An important part of our efforts is to create sufficient computer support for cost-effective course development. This is done in three ways: development of a dedicated repository system using metadata, for easy storage and retrieval of Learning Objects; creation of a tool which combines them into courses; and construction of a tool for making Learning Objects.

Design of the web-tool on differential equations. **Peep Miidla** (University of Tartu, Estonia) IC/MT3913/171

In the presentation the principles of designing of the web-tool on differential equations are considered. The main parts of the tool are: lecture notes, exercises, examples, interactive illustrative and modelling facilities, consultation network, blackboard, evaluation system and some others. These parts will be discussed and not all of them have the same weight from the teaching point of view. In some ways the open courseware system could be used, but several things are new in teaching experience. The classical course of ordinary differential equations must be supported by e-learning means and the best didactic possibility seems to be the blended learning.

The talk is based on the experience of Estonia.

Remote courses for applied mathematics at universities in sub-Saharan Africa. **Verdiana Masanja** (University of Dar es Salaam, Tanzania) IC/MT3952/171

The 1990s saw great pressure to expand student enrollment and improve education delivery with dwindling resources at most Sub-Saharan African (SSA) Higher Education Institutions (HEIs). The HEIs saw the solutions to this dilemma in the utilization of Information and Communication Technology (ICT). Many initiatives have been undertaken at many SSA HEIs to foster education and training systems through the effective and relevant use of ICTs and the Internet for learning (eLearning). Projects have been funded to explore eLearning issues such as new learning environments, virtual models of education and training, teachers' training to use ICT in education and the development of eContent. This presentation explores the extent to which such initiatives in four universities in SSA have contributed to the integration of ICT enhanced tools and services in the education and training of remote courses in Applied Mathematics and discusses the potential areas of collaboration.

IC/MP208/171: Virtual environments in applied mathematics.

Organiser: Matti Heilio (Lappeenrannan Teknillinen Yliopisto, Finland)
Co-organiser: Pietro Pantano (Università della Calabria, Italy)

Virtual technologies and digital educational environments are a viable media to support innovative processes. They can be used to bring solutions to training and educational needs, to facilitate distributed and concurrent work processes, provide remote access to software libraries and knowledge repositories. We are witnessing an evolution of educational materials from traditional textbook to interactive cross-media environments. Flexible updates, dynamic edition, easy accesss and

portability. Additional benefits come from hypermedia features. Graphical arts, animation, interactivity and visual effects of user interface are important possibilities opened by the virtual technology and web-distribution.

Topics of the talks include Remote access laboratories in applied mathematics, Art, mathematics and cultural industry, Mathematics and visualization: multi-dimensional digital shapes for e-learning, Cooperative work in a e-learning environment.

Remote access laboratories in applied mathematics. **Matti Heilio** (Lappeenrannan Teknillinen Yliopisto, Finland) IC/MT1357/171

The cutting edge knowledge in the art of mathematical technology in Europe can be located in dispersed nodes, research groups on applied mathematics, mathematical physics, scientific computing. The work of these groups often lead to development of software that represent state-of-the-art scientific knowledge in the field. These environments are often experimental, under revisions, near the laboratory floor of on-going research. This stage sometimes precedes the later development to actual products and commercialization.

Web-technologies are a viable media for innovative processes and knowledge transfer. A possibility to empower the use of mathematics is sharing of software via remote access to software libraries. In this talk I draw attention to the possibility of creating added value for the knowledge repository of applied mathematics and computational methods via remote access software sharing. To illustrate I present examples and refer to the obvious potential of this approach in the modern era of grid computing. Interactive installations created at GMD Institute for Media Communication provide high level visual support for educational purposes. Applications include illustration of string theory, virtual planetarium and topological zoo.Nondifferentiable Interactive Multiobjective BUndle-based optimization System NIMBUS has been developed at the University of Jyväskylä. The WWW interface enables remote handling of optimization problems and experimenting with up-to-date methods.Web System for Solving Diophantine Systems developed at the Petrozavodsk State University is available for distant users. Web-based system for graduate studies - Optimization, Games and Markets developed at the University of Kaunas, offers versatile collection of interactive exercises. By international collaboration the mathematics community could create a powerful service grid, a library of contemporary and proto-level scientific software in modeling, numerical methods and scientific computing.

Art, mathematics and cultural industry: new trends in the digital era. **Mauro Francaviglia** (Università degli Studi di Torino, Italy), Marcella Lorenzi (Università della Calabria, Italy), Pietro Pantano (Università della Calabria, Italy) IC/MT1377/171

Communicating fundamental achievements of Mathematics is by no means simple, so that presenting it in an innovative way is a fascinating challenge dictated by new trends of our Society. Maths and Art have developed in parallel; in our days Maths plays a renewed role in Art, out of which it gains one reason of development. Maths contributes to conceiving and shaping the World, while Art develops the means to harmonise, describe, represent aesthetically our sensations and perception. Programs aimed at developing interactions between Maths and Art belong to the broad field called Mathematics in Cultural Industry. A new way of teaching and communicating Maths should be envisaged, which requires a deeper use of the intertwining between Maths and Art. Where Art is the central theme out of which the existence of mathematical structures is recognized, first as an hidden part and later revealed more explicitly; to extract and understand structures, symmetries and broken symmetries out of their appearance within Art. To obtain new perspectives on Maths use should be done of the modern tools that new technologies provide us: Digital Technologies, Multimedia and Web Technology, in particular. The innovative full teaching project we are currently developing is mainly associated with a Web Portal MArs aimed at allowing a softer way of understanding Maths, at progressive levels of abstraction, where Art comes first and touches the emotions, stimulating the need to penetrate more intimately into the structures which underly Art. Mars will therefore present Art as a way to approach Maths, to enjoy the beautifulness of the structures existing in our vision and representation of the World and eventually to reconstruct the structures and theoretical tools that are necessary to understand and elaborate their true essence. The Portal will host less conventional spaces dedicated to: the development and/or presentation of multimedia; simulations and generative approaches to Mathematical Art; digital technologies to produce Art through Mathematics or to understand Mathematics through Art; new frontiers in Maths stimulated by Digital Art and Artificial Life, Virtual and Augmented Reality; the use of virtual frameworks and agents to make presentations of Maths (and Science in general) more attractive and artistically valid.

Multidimensional digital shapes for e-Learning. **Tor Dokken** (SINTEF, Norway), Ewald Quak (Tallinn University of Technology, Estonia) IC/MT1437/171

The use of digital shapes, either in 3D (through static models) or 4D (through the animation of 3D objects), is especially important for eLearning applications, since such shapes offer a lot of possibilities well beyond reproducing the content of a “flat" book: a molecule can be inspected from different viewpoints; medical students can make their first steps in the training for surgical procedures; 3D characters of computer games can be used for educational purposes as well.

In this talk a number of examples from European and other projects, such as the IST Network of Excellence AIM@SHAPE, will be presented to illustrate how shapes can be viewed as prime contributing factors for eLearning applications.

Cooperative work in an e-Learning environment: the COMSON case. **Valerio Talarico** (Bergische Universität Wuppertal, Germany), Pietro Pantano (Università della Calabria, Italy), Eleonora Bilotta (Università della Calabria, Italy) IC/MT2449/171

COupled Multiscale Simulation and Optimization in Nanoelectronics project is a Marie Curie RTN supported by the European Commission within the 6th Framework Research Programme of the EU. The COMSON project is run by a Consortium whose multiple aims are: to build an experimental software Demonstrator Platform for coupled simulation of devices, interconnects, circuits, EM fields and thermal effects (one single framework for simulation tool, optimisation in compound design space); to provide an e-learning platform to be used as an inter and extra consortium TOK (transfer of knowledge) infrastructure; to provide a collaborative virtual work environment (CWE) to be used both for industrial activities and training.

COMSON merges the know-how of the three major European semiconductor industries with the combined expertise of specialized university groups for developing adequate mathematical models and numerical schemes and realizing them in a CWE leveraging the demonstrator platform. On the one hand, one of the main activities is to test mathematical methods and approaches, so as to assess whether they are capable of addressing the industryŠs problems using the same CWE; on the other hand, the focus is in adequately educating young researchers by obtaining immediate hands-on experience for state-of-the-

art problems through the e-learning and CWE platform.

The COMSON CWE has been designed as a virtual working place (VWP) where each inter-actor can access different tools and facilities, based upon his/her level of expertise and role. The VWP aim is to allow easy sharing of knowledge between interactors by providing an integrated environment that permits natural communication between participants as well as intuitive exploration, discovery and use of tools based on manipulatory interfaces. The core VWP macrocomponents are:

- A 3D representation of a virtual world based on the museum metaphor used to gain access to the various sub systems.
- A 3D lab allowing users to design, share, experiment, manipulate models and systems.
- A fully featured communication facility allowing voice, video and text instant messaging everywhere in the VWP.
- Collaboration tools for knowledge sharing (e-learning), cooperative design and experiment.
- An intelligent multi agent management system to support exploration.

The VWP has been interfaced with a standardized Learning Management Content System (LMCS) and DP remote simulator. The e-learning platform uses different technologies for the preparation of high-quality e-Learning courses sing multimodal interfaces, embodied into virtual 3D agents, which produce attractive interaction with the user in order to improve and scaffold learning. According to the educational and industrial needs, these environments are designed in order to integrate different systems which improve the student skills in this specific field. This environment is an effective approach for obtaining skills in microelectronics by using different learning situations (ranging from video lessons to hands-on experiences in the DP) in which professional training can be activated also for non-specialists.

IC/MP648/015: Transferring mathematical skills and knowledge today and tomorrow: a tribute to Olga Taussky-Todd.

Organiser: Frank Uhlig (Auburn University, USA)

This mini-symposium is interdisciplinary in nature and reaches beyond applied and industrial mathematics. It deals with our innate and cultured math abilities, the role of gender, nature and nurture in learning and teaching mathematics. It is inspired by and in honor of Olga Taussky-Todd. We start with a personal assessment of Olga's influence on mathematics and mathematicians and her role as a torchbearer and teacher for math and science, followed by recent findings in math education and human neuroscience.

In this vein we first develop teaching principles that help students become autonomous math thinkers. This is based on work by G. Harel. Then we look into specific difficulties in teaching and learning linear algebra, using research by A. Sierpinska, J.-L. Dorier and others. These sets of findings both ultimately lead to and ask for curriculum changes in K–12 math teaching.

The second talk gives an exposition of recent research from cognitive psychology and neuroscience of innate math abilities in infants, as well as of the number line perception that we acquire through culture. The latter is related to space conception and specific areas and known activities of the brain. These findings can aid us to teach mathematics more appropriately. The third talk returns to the narrower subject matter of this Congress and tries to draw conclusions for applied mathematics education and applied mathematicians on what to teach students of numerical analysis and how.

Finally there will be a panel discussion of questions and comments from the floor with the presenters. The aim of this minisymposium is to open a dialogue between the applied and industrial math community and concerned math educators, cognitive psychologists, neuroscientists, and College math faculty about the challenges in teaching mathematics and ultimately to help preserve and improve the mathematical base in our culture and society.

Olga Taussky, a torchbearer for mathematics and teacher of mathematicians, and current math-education insights into general math and linear algebra teaching and learning. **Frank Uhlig** (Auburn University, USA) IC/MT4080/174

Olga Taussky-Todd's mathematical and personal life (1906–1995), her achievements and obstacles, her scientific reasoning and teaching all have served as inspiration to many mathematicians.

We describe her role in the mathematics world of the previous century as a torchbearer for mathematics and mathematicians, bearing the *torch of scientific truth* that burns inside of mathematics and its applications. Besides her many deep math contributions—too many to elaborate—she excelled at distilling and presenting mathematical concepts and ideas in her work and gave many visionary math talks. By sharing her mathematical visions freely she has inspired many of us. Her graceful example shall act as a springboard to the lectures of this minisymposium, given in her honor.

Besides discovering and solving mathematics and applications problems, a mathematician's most important task is that of a teacher of others.

What is Mathematics? How do we teach and learn math? Based on work by Guershon Harel: Math teaching encompasses subject matter and conceptual tools, as well as correct ways of thinking mathematically and proper ways of understanding. Desirable ways of thinking must be nurtured in children of all ages. This should cumulatively lead College entering students to understand *algebraic equivalence* in mathematics. Entering students must have repeatedly experienced working with one concept or math problem in several equivalent mathematical forms or in several mathematical languages. The ultimate aim for all students should be to become autonomous and spontaneous thinkers in mathematical situations, from K–12 and beyond, through postgraduate studies, depending on the age level, of course.

Next we describe some recent results of A. Sierpinska, J.-L. Dorier, and others on teaching and learning Linear Algebra, one of Olga Taussky's beloved subjects. Linear Algebra uses three separate languages as tools for understanding: a geometric one, an algebraic one, and an abstract, conceptual one. All interchangeably, with associated difficulties for students and teachers. Most of our students have only experienced concrete, practical thinking and have no practise with abstract, theoretical, or conceptual thinking. However, the abstract language of Linear Algebra is essential to form correct concept images and thereby gain correct ways of understanding and thinking. To achieve this, teachers of a Linear Algebra course need to allow and encourage constant shifts in language and viewpoint of the subject matter so that students become conscious and flexible in order to achieve autonomous thoughts in math.

Is abstract thinking necessary for Linear Algebra? This leads to deeper questions:Is abstract, theoretical thinking needed in math and applied math? Can we do without scientific knowledge and exploration in Academia, or is practical knowledge alone sufficient?

To prepare students for scientific exploration in College requires changes in our K–12 curricula so that theoretical thinking is practised from early age on, and repeatedly, and becomes natural throughout College and beyond.

Can cognitive neuroscience influence math education?. **Edward Hubbard** (INSERM, France) IC/MT4102/174

Over the past twenty years a variety of experiments have converged to demonstrate that adult human numerical and mathematical abilities are based on evolutionarily conserved and developmentally precocious mechanisms. This talk briefly reviews some research results that show striking numerical competencies in both non-human primates and in human infants.

Building on these results, I will discuss current cognitive neuroscience research on the notion of a "mental number line." For example, it is well established that subjects compare two numbers more quickly when the distance between them is large (such as 55 and 94) than when the distance is small (e.g., 55 and 47). Neuroimaging studies have shown that the human ability to compare numbers depends on a part of the brain known as the intraparietal sulcus. Structural imaging studies have found anatomical differences in this region of the brain in children with severe developmental difficulties in math.

As regards the spatial representation of numbers, which in Western culture (writing from left to right) is a mental mapping of small numbers to the left side and of large numbers to the right side, neuroimaging studies show that these abilities depend on regions of the brain involved in our spatial abilities.

Finally, I will propose some specific examples that show how these findings could aid us when teaching mathematics.

How and why should we teach numerical analysis?. **Anne Greenbaum** (University of Washington, USA) IC/MT4209/174

The field of numerical analysis can include: the design, analysis, and computer implementation of algorithms; the use of these algorithms in applications from science and engineering to finance to the internet to video games and computer graphics.
Which of these areas should be emphasized in an introductory numerical analysis course? Applications can be *glitzy*, but if they are introduced without the requisite understanding of the algorithms being used, they run the risk of providing entertainment without much actual learning. On the other hand, convergence proofs can be boring, especially if one has just been introduced to an algorithm and one wants to get a feel for how it works before studying it in depth. Finding the right mix of these ingredients is a challenge for current teachers of numerical analysis, and for anyone trying to convey the importance and mathematical beauty of this field.

In this talk, we discuss some ways of balancing the different aspects and how well or poorly they seem to be working. Of course, measuring how well something works presupposes that one knows what one wants to accomplish. What should the goals of an introductory numerical analysis course be and how do we go about accomplishing those goals? The answers may depend on one's perspective, be it academic or industrial, engineer or biologist or movie maker.

Still there should be some general principles that all can agree on. We discuss possible goals and student expectations as well.

Panel discussion of audience questions and comments. **Frank Uhlig** (Auburn University, USA), Edward Hubbard (INSERM, France), Anne Greenbaum (University of Washington, USA) IC/MT4570/174

We shall discuss topics from mathematical education, human math abilities, and the role of math teachers, students and curricula with the audience.

17: Education Culture and History, Contributed Talks

17: Education Culture and History, Posters

IC/PP2425/017: **Mathematical notation and the use of functions.**

Presenter: Henning Thielemann (Universität Halle-Wittenberg, Germany)

In contrast to natural languages, mathematical notation is accepted as being exceptionally precise. It shall make mathematical statements unambiguous, it shall allow formal manipulation, it is model for programming languages, computer algebra systems and machine provers. However, what is "mathematical notation" today and is it indeed as precise as expected?

On the poster we discuss some examples of notation which require caution. How are they adapted in computer algebra systems? Can we replace them by something less problematic? What can we learn from functional programming?

IC/PP4393/172: **Teaching mathematics to engineers with *Mathematica*.**

Presenter: Conchita Marin (Universidad de Extremadura, Spain)

Over last years, increasing using of informatics tools on education is absolutely generalized, in particular, interesting mathematics software with large-scale applications has been developed. It has been proved, they are a very good help on learning not only because rapid calculations are possible, but because they let students to reach concepts in a clearer way. Moreover, in the formation of a future engineer, it is important to get him a correct and fluent interpretation of numerical results. On other hand, they should be able to design their own programs to solve problems. In this sense, using any kind of mathematical software integrating numeric and symbolic computation will be a no discussible help. In this work, academic results of students learning with Mathematica are analyzed. This software was used to teach "Numeric Calculus", an optional subject which students can choose from his second year on the university, so that, all of them have already attended to a course on Mathematics Fundaments of Engineer at his first year. The number of students was never more than twenty five in order to get a good evaluation of the efficiency of the methodology employed. The results correspond to the last five years in an Engineer School.